Weak variations of Lipschitz graphs and stability of phase boundaries

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Cont. Mech. Thermodyn., Vol. 23, no. 2 (2011) pp. 87–123

Abstract

In the case of Lipschitz extremals of vectorial variational problems an important class of strong variations originates from smooth deformations of the corresponding non-smooth graphs. These seemingly singular variations, which can be viewed as combinations of weak inner and outer variations, produce directions of differentiability of the functional and lead to singularity-centered necessary conditions on strong local minima: an equality, arising from stationarity, and an inequality, implying configurational stability of the singularity set. To illustrate the underlying coupling between inner and outer variations we study in detail the case of smooth surfaces of gradient discontinuity representing, for instance, martensitic phase boundaries in nonlinear elasticity.

Contents

1 Introduction

Equilibria in continuum mechanics are usually identified with strong local minima of integral functionals. Classical Calculus of Variations supplies the well known necessary conditions of strong local minimum [19] that are basically sufficient in the case of smooth extremals [24, 25]. The smoothness of extremals, however, is not certain when the Lagrangian is smooth. Even if conditions of convexity and coercivity are added, the Lipschitz continuity of extremals cannot be guaranteed [54, 59]. In elasticity theory convexity is excluded by frame indifference, and it is not uncommon to encounter non rank one convex functionals, as in the case of martensitic materials or in shape optimization problems. Smooth extremals in such theories are exceptions and the systematic treatment of singularities becomes essential. The most well-known examples of singular minimizers are elastic equilibria where coexisting phases are separated by phase boundaries (e.g. [47, 6]). For the general discussion of singular extremals in the Calculus of Variations we refer to [60, 9, 19], the Continuum Mechanics perspective can be found in [41, 50, 31, 4, 5].

The C^0 topology in the notion of strong minimization is compatible with variations of the singularity sets. It is therefore necessary to look for additional, singularity centered, necessary conditions of equilibrium and stability. In connection with this we can mention partial regularity results for global and strong local minima [14, 36] for uniformly quasiconvex energies. For Lipschitz extremals of general energies there exist strong variations of special type, corresponding to weak variations of their graphs. In this paper we show that such seemingly singular variations produce directions of differentiability of the functional along which both the first and the second variations can be computed. The resulting necessary conditions can be used to test the configurational stability of the singularity set.

An important example of Lipschitz singularities is a smooth surface of jump discontinuity of the gradient $\nabla \boldsymbol{y}(\boldsymbol{x})$. Such singularities are encountered in a variety of applications. For instance, the optimal Vigdergauz microstructures [56, 57, 58] emerge as minimizers in the theory of shape optimization [22, 20]. Two phase precipitates in metallurgy and material science represent stable inclusion-type configurations [33, 16]. In addition, Lipschitz type "classical designs" and "finite scale microstructures" are typical features of the regularized theories.

Engineering studies of mechanical instabilities associated with smooth external and internal surfaces of discontinuity, initiated in [55, 7], were mostly focused on *weak* local minimizers and the corresponding mathematical results can be found in [53, 40, 49, 50, 42]. For *strong* local minimization, the study of first order stability conditions on jump discontinuities was initiated by Weierstrass (see [11, 18]). In the case of phase transitions between nonlinear elastic phases the first variation was studied by Eshelby [13] (see also [48, 27, 32]) while the second variation was first computed by Grinfeld [28] (see also [35, 3, 37, 17]).

In this paper we formulate the global necessary conditions of stability and re-examine Grinfeld's pioneering results from the general perspective of Calculus of Variations. In particular, we study in full detail the localized version of the stability conditions and derive explicit algebraic inequalities generalizing all previously known local conditions of morphological instability for smooth surfaces of gradient discontinuity (e.g.[28, 53, 37]). For simplicity we keep the outer domain fixed disabling the corresponding boundary surface instabilities.

The paper is organized as follows. We begin with an heuristic discussion of the main ideas of the paper in Section 2. In Section 3 we derive the explicit expressions for the first and second mixed inner-outer variations in a form applicable to *general* Lipschitz extremals. In Section 4 we prove that for smooth extremals the mixed inner-outer variations can always be reduced to outer variations. We then formulate the idea of Euler-Lagrange equivalence (EL equivalence) representing a weaker version of Noether's variational symmetry. The extremals with smooth surfaces of jump discontinuities are considered in Section 5 where we apply our general results to derive explicit expressions for the first and second variations. The global necessary conditions are formulated in Section 6 where we also discuss singularities of higher co-dimension. In an illustrative example we show that the global stability condition can detect instabilities which would be missed by the corresponding local conditions. The global conditions are localized and reduced to a set of algebraic inequalities in Section 7. To illustrate the local necessary conditions we provide another example where the singularity centered algebraic conditions detect an instability, that the classical second variation misses.

In this paper we use index-free notation, whenever possible. The subscripts like $L_{\boldsymbol{F}}$ denote the matrices of partial derivatives $\partial L/\partial F_{ij}$. We use the inner product notation $(\boldsymbol{a}, \boldsymbol{b})$ to denote the dot product of two vectors or a Frobenius inner product $\mathrm{Tr}\,(\boldsymbol{A}\boldsymbol{B}^T)$ of two matrices. In most cases we are able to deal with multi-index arrays by using the convention that $(\nabla\boldsymbol{A})\boldsymbol{b}$ denotes (in Einstein's notation) $A_{ij\ldots k,\alpha}b^{\alpha}$.

2 Preliminaries

Let Ω be an open and bounded domain in $\mathbb{R}^d$ with Lipschitz boundary. In this paper we study some of the conditions necessary for a Lipschitz function $\boldsymbol{y} : \Omega \to \mathbb{R}^m$ to be a local minimizer of the integral functional

$$I(\boldsymbol{y})=\int_{\Omega}L(\boldsymbol{x},\boldsymbol{y},\nabla\boldsymbol{y})d\boldsymbol{x}, \tag{2.1}$$

subject to specified boundary conditions. A fairly common type of boundary conditions imposes linear constraints on the boundary values of $\boldsymbol{y}(\boldsymbol{x})$. In other words, we assume that

$$\boldsymbol{y}\in\overline{\boldsymbol{y}}+\mathrm{Var}, \tag{2.2}$$

where $\overline{\boldsymbol{y}}$ is a given Lipschitz function and Var is a subspace of $W^{1,\infty}(\Omega;\mathbb{R}^m)$, containing $W_0^{1,\infty}(\overline{\Omega};\mathbb{R}^m)$. Therefore, the subspace Var is described in terms of linear constraints on the boundary values only. We assume that the Lagrangian $L(\boldsymbol{x},\boldsymbol{y},\boldsymbol{F})$ is jointly continuous in its variables and of class C^2 on an open neighborhood $\mathcal{U}$ of the set[1] $\mathcal{R}=\{(\boldsymbol{x},\boldsymbol{y}(\boldsymbol{x}),\nabla\boldsymbol{y}(\boldsymbol{x})):\boldsymbol{x}\in\overline{\Omega}\}$.

Let us recall the classical notions of weak and strong local minima.

Definition 2.1. *We call $\boldsymbol{y}(\boldsymbol{x})$ a strong local minimizer if $I(\boldsymbol{y}+\boldsymbol{\phi}_n)\geq I(\boldsymbol{y})$ for all n large enough and for all sequences $\{\boldsymbol{\phi}_n\}\subset\mathrm{Var}$ such that $\boldsymbol{\phi}_n\to\mathbf{0}$ uniformly as $n\to\infty$. We call $\boldsymbol{y}(\boldsymbol{x})$ a weak local minimizer if $I(\boldsymbol{y}+\boldsymbol{\phi}_n)\geq I(\boldsymbol{y})$ for all n large enough and for all sequences $\{\boldsymbol{\phi}_n\}\subset\mathrm{Var}$ such that $\boldsymbol{\phi}_n\to\mathbf{0}$ in the $W^{1,\infty}$ norm.*

We observe that strong local minimizers are stable with respect to strong and weak variations, while weak local minimizers are stable with respect to only weak variations.

Definition 2.2. *We call a sequence $\{\boldsymbol{\phi}_n\}\subset\mathrm{Var}$ a strong variation if $\boldsymbol{\phi}_n\to\mathbf{0}$ uniformly as $n\to\infty$, while $\nabla\boldsymbol{\phi}_n$ does not converge to zero uniformly. A weak variation is a sequences $\{\boldsymbol{\phi}_n\}\subset\mathrm{Var}$ such that $\boldsymbol{\phi}_n\to\mathbf{0}$ in the $W^{1,\infty}$ norm.*

A typical strong variation is the generalized Weierstrass needle

$$\boldsymbol{y}(\boldsymbol{x})\mapsto\boldsymbol{y}(\boldsymbol{x})+\epsilon\boldsymbol{\zeta}((\boldsymbol{x}-\boldsymbol{x}_0)/\epsilon),\qquad\boldsymbol{\zeta}\in C_0^1(B(\mathbf{0},1);\mathbb{R}^m). \tag{2.3}$$

In classical elasticity theory the variations (2.3) are often associated with nucleation phenomena (e.g. [2]).

A typical weak variation is the outer variation of the form

$$\boldsymbol{y}(\boldsymbol{x})\mapsto\boldsymbol{y}(\boldsymbol{x})+\epsilon\boldsymbol{\phi}(\boldsymbol{x}),\qquad\boldsymbol{\phi}\in\mathrm{Var}. \tag{2.4}$$

The most important difference between the weak and the strong variations is that the functional $I(\boldsymbol{y})$ is differentiable on weak variations and non-differentiable on strong ones. Indeed, in the case of weak variations the directional derivative

$$D_{\boldsymbol{\phi}}I=\lim_{\epsilon\to0}\frac{I(\boldsymbol{y}+\epsilon\boldsymbol{\phi}(\boldsymbol{x}))-I(\boldsymbol{y})}{\epsilon}$$

[1] The set $\mathcal{R}$ is compact, when $\boldsymbol{y}(\boldsymbol{x})$ is of class C^1. In the general case we mean the closure of the set of Lebesgue points of the measurable set $\mathcal{R}$.

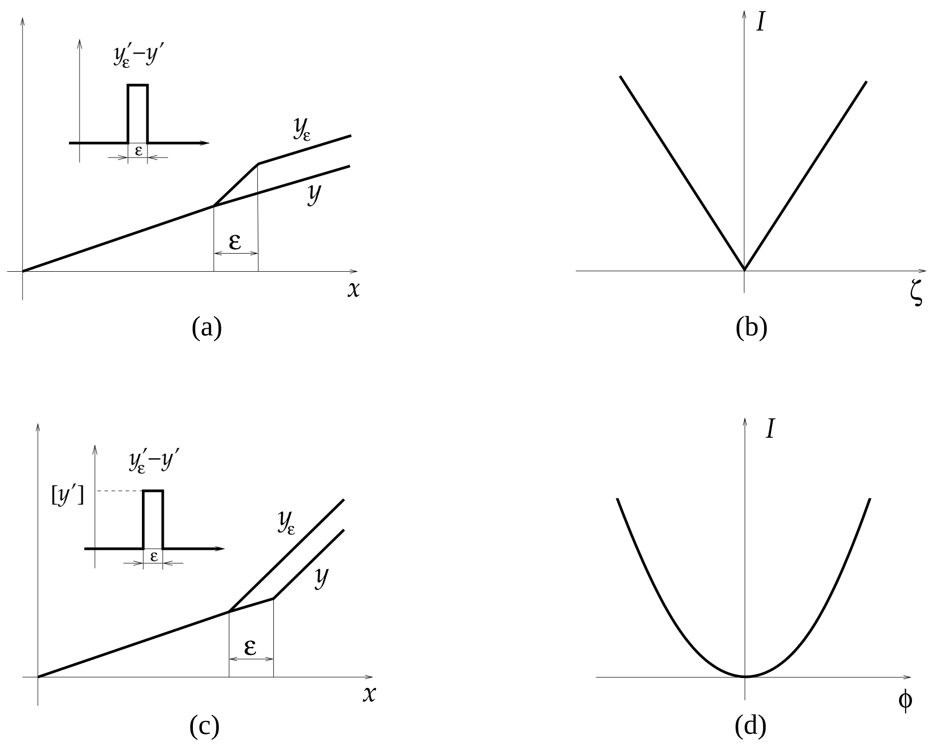

Figure 1: (a,b) Classical Weierstrass needle variation (nucleation) leading to necessary conditions in the form of inequalities. (c,d) Weak variation of a Lipschitz graph representing configurational shift in the location of a defect and leading to necessary conditions in the form of both equalities and inequalities.

is linear in $\boldsymbol{\phi}$. At the same time the appropriate "directional derivative" for the case of strong variations,

$$D_{\boldsymbol{\zeta}} I = \lim_{\epsilon \to 0} \frac{I(\boldsymbol{y} + \epsilon \boldsymbol{\zeta}((\boldsymbol{x} - \boldsymbol{x}_0)/\epsilon)) - I(\boldsymbol{y})}{\epsilon^d}$$

is non-linear in $\boldsymbol{\zeta}$. Therefore, the associated local minimization conditions are of two different types: equalities and inequalities, repsectively.

Below, to illustrate the difference between these two types of variations we first obtain the conditions of vanishing of the first derivative $D_{\boldsymbol{\phi}} I$ and non-negativity of the second derivative $D_{\boldsymbol{\phi}\boldsymbol{\phi}} I$ in the differentiable directions $\boldsymbol{\phi}(\boldsymbol{x})$. Then, we obtain the quasiconvexity inequality $D_{\boldsymbol{\zeta}} I \geq 0$ along the non-differentiable "directions" $\boldsymbol{\zeta}((\boldsymbol{x} - \boldsymbol{x}_0)/\epsilon)$ (see Figure 1(b)).

When $\boldsymbol{y}(\boldsymbol{x})$ is a C^1 extremal, the two types of variations are independent [24, 25], while for Lipschitz local minimizers, the situation is more complex. The weak variations of the graph of $\boldsymbol{y}(\boldsymbol{x})$ is a strong variation $\{\boldsymbol{\phi}_\epsilon\}$, for which the functional increment $I(\boldsymbol{y}+\boldsymbol{\phi}_\epsilon)-I(\boldsymbol{y})$ exhibits the differentiability properties characteristic of weak variations (see Figure 1(d)). The existence of such strong variations suggests that in the Lipschitz case the partition of variations into the weak and the strong is no longer appropriate and that some strong variations can also generate necessary conditions in the form of equalities.

The weak variations of Lipschitz graphs are defined as follows. The graph of $\boldsymbol{y}(\boldsymbol{x})$ is the set $\Gamma_{\boldsymbol{y}} = \{(\boldsymbol{x}, \boldsymbol{y}(\boldsymbol{x})) : \boldsymbol{x} \in \Omega\} \subset \mathbb{R}^d \times \mathbb{R}^m$. The weak variation of the graph is the "perturbed graph"

$$\Gamma_{\boldsymbol{y}_\epsilon} = \{(\boldsymbol{x} + \epsilon\boldsymbol{\theta}(\boldsymbol{x}), \boldsymbol{y}(\boldsymbol{x}) + \epsilon\boldsymbol{\phi}(\boldsymbol{x})) : \boldsymbol{x} \in \Omega\}, \tag{2.5}$$

where $\boldsymbol{\phi} \in \mathrm{Var} \cap C^2(\overline{\Omega}; \mathbb{R}^m)$ and $\boldsymbol{\theta} \in C^1(\overline{\Omega}; \mathbb{R}^d) \cap C_0(\Omega; \mathbb{R}^d)$. Obviously, $\Gamma_{\boldsymbol{y}_\epsilon}$ is the graph of

$$\boldsymbol{y}_\epsilon(\boldsymbol{x}) = \boldsymbol{y}(\boldsymbol{\vartheta}_\epsilon(\boldsymbol{x})) + \epsilon\boldsymbol{\phi}(\boldsymbol{\vartheta}_\epsilon(\boldsymbol{x})), \quad \boldsymbol{x} \in \Omega, \tag{2.6}$$

where $\boldsymbol{\vartheta}_\epsilon(\boldsymbol{x})$ is the inverse map of $\boldsymbol{x} + \epsilon\boldsymbol{\theta}(\boldsymbol{x})$. Hence, weak variations of Lipschitz graphs can be represented as a combination of inner and outer variations, where the inner variation is defined by

$$\boldsymbol{y}(\boldsymbol{x}) \mapsto \boldsymbol{y}(\boldsymbol{\vartheta}_\epsilon(\boldsymbol{x})). \tag{2.7}$$

More general classes of variations were considered in [15].

A weak variation of the graph, illustrated schematically in Figure 1(c) shows that the total outer variation (the Eulerian image of the combined inner-outer variation)

$$\boldsymbol{\phi}_\epsilon(\boldsymbol{x}) = \boldsymbol{y}(\boldsymbol{\vartheta}_\epsilon(\boldsymbol{x})) + \epsilon\boldsymbol{\phi}(\boldsymbol{\vartheta}_\epsilon(\boldsymbol{x})) - \boldsymbol{y}(\boldsymbol{x}). \tag{2.8}$$

is indistinguishable from the Weierstrass needle shown in the inset of Figure 1(a). More precisely, $\nabla\boldsymbol{\phi}_\epsilon$ is small everywhere, except on the set of small measure localized near the defects of $\nabla\boldsymbol{y}(\boldsymbol{x})$. In classical elasticity theory such variations are often identified with configurational displacements of crystal defects (propagation).

We now turn to the question of stability of the functional (2.1) with respect to weak variations of the graph of the Lipschitz map $\boldsymbol{y}(\boldsymbol{x})$. The functional increment $I(\boldsymbol{y}_\epsilon) - I(\boldsymbol{y})$, corresponding to the weak variation of the graph is, at the first glance, not differentiable, confirming the strong variation picture. However, the change of variables $\boldsymbol{z} = \boldsymbol{\vartheta}_\epsilon(\boldsymbol{x})$ gives

$$I(\boldsymbol{y}_\epsilon) = \int_\Omega L\left(\boldsymbol{z} + \epsilon\boldsymbol{\theta}(\boldsymbol{z}), \boldsymbol{y}(\boldsymbol{z}) + \epsilon\boldsymbol{\phi}(\boldsymbol{z}), \boldsymbol{F}(\boldsymbol{z})(\boldsymbol{I} + \epsilon\nabla\boldsymbol{\theta})^{-1} + \epsilon\nabla\boldsymbol{\phi}\right) \det(\boldsymbol{I} + \epsilon\nabla\boldsymbol{\theta}) d\boldsymbol{z}, \tag{2.9}$$

where $\boldsymbol{F}(\boldsymbol{x})$ is our notation for the gradient $\nabla\boldsymbol{y}(\boldsymbol{x})$. It is now obvious that $I(\boldsymbol{y}_\epsilon)$ depends in a smooth way on $\boldsymbol{\theta}$ and $\boldsymbol{\phi}$, even when $\boldsymbol{F}(\boldsymbol{x})$ is merely measurable and bounded. Observe that the inner and outer variations play very different roles. The former affects Lagrangian variables $\boldsymbol{x}$ and moves singularities, while the latter perturbs the Eulerian variables $\boldsymbol{y}$ and preserves the locations of singularities. One can see that in the Lipschitz case neither the first variation nor the the second can be fully understood in terms of the inner or outer variations alone.

If $\boldsymbol{y}(\boldsymbol{x})$ is of class C^1 then there are no singularities to move and (2.6) is equivalent to the pure outer variation (2.4). Indeed, using the Taylor expansion

$$\boldsymbol{\vartheta}_\epsilon(\boldsymbol{x}) = \boldsymbol{x} - \epsilon\boldsymbol{\theta}(\boldsymbol{x}) + o(\epsilon),$$

we obtain,

$$\boldsymbol{y}_\epsilon(\boldsymbol{x}) = \boldsymbol{y}(\boldsymbol{x}) - \epsilon\boldsymbol{F}(\boldsymbol{x})\boldsymbol{\theta}(\boldsymbol{x}) + \epsilon\boldsymbol{\phi}(\boldsymbol{x}) + o(\epsilon).$$

Hence,

$$\boldsymbol{y}_\epsilon(\boldsymbol{x}) = \boldsymbol{y}(\boldsymbol{x}) + \epsilon\boldsymbol{\psi}(\boldsymbol{x}) + o(\epsilon), \tag{2.10}$$

where $\boldsymbol{\psi}(\boldsymbol{x})$ is given by

$$\boldsymbol{\psi}(\boldsymbol{x}) = \boldsymbol{\phi}(\boldsymbol{x}) - \boldsymbol{F}(\boldsymbol{x})\boldsymbol{\theta}(\boldsymbol{x}). \tag{2.11}$$

This shows that when $\boldsymbol{y} \in C^1(\overline{\Omega}; \mathbb{R}^m)$ the inner-outer variation (2.6) is equivalent to the outer variation (2.4), with $\boldsymbol{\phi}$ replaced by $\boldsymbol{\psi}$, given by (2.11). This leads us to the notion of the EL (Euler-Lagrange) equivalence, discussed in detail in Section 4.1, which can also be regarded as a variational symmetry.

Remark 2.3. *There is an important difference between the inner and outer variations. The inner variations can only produce outer variations of the form*

$$\boldsymbol{\phi}(\boldsymbol{x}) = -\boldsymbol{F}(\boldsymbol{x})\boldsymbol{\theta}(\boldsymbol{x}) \tag{2.12}$$

If $\boldsymbol{F}(\boldsymbol{x}) = \nabla\boldsymbol{y}(\boldsymbol{x})$ is a rectangular matrix, or a singular square matrix, then the equation (2.12) may not be solvable for $\boldsymbol{\theta}$. In addition, in our setting, the outer variations that are equivalent to the inner ones must necessarily vanish on $\partial\Omega$.

When singularities of the gradient $\boldsymbol{F}(\boldsymbol{x})$ are present the symmetry is broken, since in the space of labels (Lagrangian coordinates) the points on the singular set are distinguished from all the other points. Nevertheless, we may extend the idea of EL equivalence, to the case when $\boldsymbol{F}(\boldsymbol{x})$ is not smooth, if we study the equivalent outer variation (2.8) corresponding to the inner-outer variation (2.6). The known structure of singularities of $\boldsymbol{F}(\boldsymbol{x})$ can then be translated into the understanding of the geometry of the set, where $|\nabla\boldsymbol{\phi}_\epsilon|$ is not small.

Our most detailed results are obtained for smooth surfaces of gradient jump discontinuity, representing, for instance, elastic phase boundaries, where the structure of the singularity is the simplest. We also show that the defects of co-dimension higher than 1 are "invisible" to our functional. The physical defects with higher co-dimension, describing for instance dislocations, crack tips and vacancies, correspond to non-Lipschitz maps which are in principle amenable to our general approach while requiring a special treatment of unbounded deformation gradients.

3 General first and second variations

The inner-outer first and second variations are defined as the derivatives

$$\delta I_\Omega(\boldsymbol{\phi}, \boldsymbol{\theta}) = \left.\frac{dI(\boldsymbol{y}_\epsilon)}{d\epsilon}\right|_{\epsilon=0}, \qquad \delta^2 I_\Omega(\boldsymbol{\phi}, \boldsymbol{\theta}) = \left.\frac{d^2 I(\boldsymbol{y}_\epsilon)}{d\epsilon^2}\right|_{\epsilon=0}$$

that can be computed in a straightforward way by differentiating under the integral in (2.9). Attempting to perform the calculations, one quickly discovers that the direct way is very tedious, at least as far as the second variation is concerned. The formalism presented below brings a transparent structure to the results and allows one to accelerate the computations considerably.

3.1 Outer and inner variation operators

We define the global outer variation operator by

$$\mathfrak{O}[\epsilon\boldsymbol{\phi}]I(\boldsymbol{y}) = I(\boldsymbol{y} + \epsilon\boldsymbol{\phi}) \tag{3.1}$$

We also define the corresponding infinitesimal outer variation operators

$$(\delta_o[\boldsymbol{\phi}]L)(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{F}) = (L_{\boldsymbol{y}}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{F}), \boldsymbol{\phi}(\boldsymbol{x})) + (\boldsymbol{P}, \nabla\boldsymbol{\phi}(\boldsymbol{x}))$$

and

$$\Delta_o[\boldsymbol{\phi}]I(\boldsymbol{y}) = \int_\Omega (\delta_o[\boldsymbol{\phi}]L)(\boldsymbol{x}, \boldsymbol{y}(\boldsymbol{x}), \nabla\boldsymbol{y}(\boldsymbol{x}))d\boldsymbol{x}, \tag{3.2}$$

where

$$\boldsymbol{P} = L_{\boldsymbol{F}}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{F})$$

is known in the context of elasticity theory as the Piola-Kirchhoff stress tensor.

We can expand the global outer variation operator $\mathfrak{O}[\epsilon\boldsymbol{\phi}]$ in powers of ϵ, even when $\boldsymbol{y}(\boldsymbol{x})$ is merely Lipschitz continuous.

LEMMA **3.1.** *Suppose* $\boldsymbol{\phi} \in W^{1,\infty}(\Omega; \mathbb{R}^m)$. *Then*

$$\mathfrak{O}[\epsilon\boldsymbol{\phi}]I(\boldsymbol{y}) = I(\boldsymbol{y}) + \epsilon\Delta_o[\boldsymbol{\phi}]I(\boldsymbol{y}) + \frac{\epsilon^2}{2}\Delta_o^2[\boldsymbol{\phi}]I(\boldsymbol{y}) + o(\epsilon^2),$$

where

$$\Delta_o^2[\boldsymbol{\phi}]I(\boldsymbol{y}) = \Delta_o[\boldsymbol{\phi}](\Delta_o[\boldsymbol{\phi}]I(\boldsymbol{y})).$$

Proof. One way to prove the lemma is to perform the explicit differentiation in (2.9) and compare the result with the expansion in the lemma. There is, however, a more enlightening proof. Let $f(\epsilon) = \mathfrak{O}[\epsilon\boldsymbol{\phi}]I(\boldsymbol{y})$. Our goal is to derive the formula for $f''(0)$ in the Taylor expansion

$$f(\epsilon) = f(0) + \epsilon f'(0) + \frac{\epsilon^2}{2}f''(0) + o(\epsilon^2)$$

without having to differentiate (2.9) twice. The idea is is to compute the *first order* expansion

$$T(\epsilon, \delta) = f(\epsilon) + \delta f'(\epsilon)$$

of $f(\epsilon + \delta)$, regarding ϵ as fixed. If we then expand $T(\epsilon, \delta)$ to *first order* in ϵ, then we obtain

$$f(\epsilon + \delta) \sim f(0) + (\epsilon + \delta)f'(0) + \epsilon\delta f''(0). \tag{3.3}$$

Hence, $f''(0)$ can be computed as the coefficient of $\epsilon\delta$ in (3.3). To prove the lemma, it remains to observe that

$$f(\epsilon + \delta) = \mathfrak{O}[\delta\boldsymbol{\phi}](\mathfrak{O}[\epsilon\boldsymbol{\phi}]I(\boldsymbol{y})).$$

Therefore,

$$T(\epsilon, \delta) = \mathfrak{O}[\epsilon\boldsymbol{\phi}]I(\boldsymbol{y}) + \delta\Delta_o[\boldsymbol{\phi}](\mathfrak{O}[\epsilon\boldsymbol{\phi}]I(\boldsymbol{y})).$$

Expanding $T(\epsilon, \delta)$ to first order in ϵ we obtain $f''(0) = \Delta_o^2[\boldsymbol{\phi}]I(\boldsymbol{y})$. ∎

Performing explicit calculations, we also obtain

$$\delta_o^2[\boldsymbol{\phi}]L = (L_{\boldsymbol{yy}}\boldsymbol{\phi}, \boldsymbol{\phi}) + (L_{\boldsymbol{FF}}\nabla\boldsymbol{\phi}, \nabla\boldsymbol{\phi}) + 2(L_{\boldsymbol{Fy}}\boldsymbol{\phi}, \nabla\boldsymbol{\phi}). \tag{3.4}$$

We define the global inner variation operator by

$$\mathfrak{I}[\epsilon\boldsymbol{\theta}]I(\boldsymbol{y}) = I(\boldsymbol{y}(\boldsymbol{\vartheta}_\epsilon)). \tag{3.5}$$

We also define the corresponding infinitesimal inner variation operators

$$(\delta_i[\boldsymbol{\theta}]L)(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{F}) = (L_{\boldsymbol{x}}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{F}), \boldsymbol{\theta}(\boldsymbol{x})) + (\boldsymbol{P}^*(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{F}), \nabla\boldsymbol{\theta}(\boldsymbol{x}))$$

and

$$\Delta_i[\boldsymbol{\theta}]I(\boldsymbol{y}) = \int_\Omega (\delta_i[\boldsymbol{\theta}]L)(\boldsymbol{x}, \boldsymbol{y}(\boldsymbol{x}), \nabla\boldsymbol{y})d\boldsymbol{x}, \tag{3.6}$$

where

$$\boldsymbol{P}^* = L\boldsymbol{I} - \boldsymbol{F}^T L_{\boldsymbol{F}} \tag{3.7}$$

is the energy-momentum tensor known in elasticity theory as the Eshelby tensor. We remark, that even though $\nabla(\boldsymbol{y}(\boldsymbol{\vartheta}_\epsilon))$ is *not* uniformly close to $\nabla\boldsymbol{y}(\boldsymbol{x})$, the formula $\nabla(\boldsymbol{y}(\boldsymbol{\vartheta}_\epsilon)) = \boldsymbol{F}(\boldsymbol{\vartheta}_\epsilon)\nabla\boldsymbol{\vartheta}_\epsilon$ shows that $(\boldsymbol{x}, \boldsymbol{y}(\boldsymbol{\vartheta}_\epsilon), \nabla(\boldsymbol{y}(\boldsymbol{\vartheta}_\epsilon)))$ stays in the set $\mathcal{U}$ (the set where the Lagrangian L is C^2) for almost all $\boldsymbol{x} \in \Omega$, since $\boldsymbol{\vartheta}_\epsilon(\boldsymbol{x})$ and $\nabla\boldsymbol{\vartheta}_\epsilon$ are uniformly close to $\boldsymbol{x}$ and $\boldsymbol{I}$, respectively. Hence, there is no problem expanding $\mathfrak{I}[\epsilon\boldsymbol{\theta}]I(\boldsymbol{y})$ in powers of ϵ even when $\boldsymbol{y}(\boldsymbol{x})$ is merely Lipschitz continuous.

Lemma **3.2.** *Suppose* $\boldsymbol{\theta} \in C^2(\overline{\Omega}; \mathbb{R}^d)$

$$\mathfrak{I}[\epsilon\boldsymbol{\theta}]I(\boldsymbol{y}) = I(\boldsymbol{y}) + \epsilon\Delta_i[\boldsymbol{\theta}]I(\boldsymbol{y}) + \frac{\epsilon^2}{2}(\Delta_i^2[\boldsymbol{\theta}] - \Delta_i[(\nabla\boldsymbol{\theta})\boldsymbol{\theta}])I(\boldsymbol{y}) + o(\epsilon^2),$$

where

$$\Delta_i^2[\boldsymbol{\theta}]I(\boldsymbol{y}) = \Delta_i[\boldsymbol{\theta}](\Delta_i[\boldsymbol{\theta}]I(\boldsymbol{y})).$$

Proof. We follow the same strategy as in the proof of Lemma 3.1. Let $f(\epsilon) = \mathfrak{I}[\epsilon\boldsymbol{\theta}]I(\boldsymbol{y})$. First we expand

$$\boldsymbol{\vartheta}_{\epsilon+\delta}(\boldsymbol{x}) = \boldsymbol{\vartheta}_\epsilon(\boldsymbol{x}) - \delta(\boldsymbol{I} + \epsilon\nabla\boldsymbol{\theta}(\boldsymbol{\vartheta}_\epsilon(\boldsymbol{x})))^{-1}\boldsymbol{\theta}(\boldsymbol{\vartheta}_\epsilon(\boldsymbol{x})) + O(\delta^2).$$

Therefore, comparing the first order expansions in δ we conclude that

$$f(\epsilon + \delta) = \mathfrak{I}[\delta\boldsymbol{\eta}_\epsilon](\mathfrak{I}[\epsilon\boldsymbol{\theta}]I(\boldsymbol{y})) + O(\delta^2),$$

where $\boldsymbol{\eta}_\epsilon(\boldsymbol{x}) = \boldsymbol{\theta}(\boldsymbol{\vartheta}_\epsilon(\boldsymbol{x}))$. Hence,

$$T(\epsilon, \delta) = \mathfrak{I}[\epsilon\boldsymbol{\theta}]I(\boldsymbol{y}) + \delta\Delta_i[\boldsymbol{\eta}_\epsilon](\mathfrak{I}[\epsilon\boldsymbol{\theta}]I(\boldsymbol{y})).$$

Expanding $T(\epsilon, \delta)$ to first order in ϵ, using

$$\boldsymbol{\eta}_\epsilon(\boldsymbol{x}) = \boldsymbol{\theta}(\boldsymbol{x}) - \epsilon(\nabla\boldsymbol{\theta}(\boldsymbol{x}))\boldsymbol{\theta}(\boldsymbol{x}) + O(\epsilon^2),$$

we obtain the lemma. □

Performing explicit calculations, we also obtain

$$\delta_i^2[\boldsymbol{\theta}]L = L((\nabla\cdot\boldsymbol{\theta})^2 - \mathrm{Tr}\,(\nabla\boldsymbol{\theta})^2) + (\boldsymbol{P}^*, \nabla((\nabla\boldsymbol{\theta})\boldsymbol{\theta})) + (L_{\boldsymbol{x}}, (\nabla\boldsymbol{\theta})\boldsymbol{\theta}) + 2(L_{\boldsymbol{x}}, \boldsymbol{\theta})\nabla\cdot\boldsymbol{\theta}$$
$$+ 2(\boldsymbol{P}, \boldsymbol{F}\nabla\boldsymbol{\theta}(\nabla\boldsymbol{\theta} - (\nabla\cdot\boldsymbol{\theta})\boldsymbol{I})) + (L_{\boldsymbol{FF}}\boldsymbol{F}\nabla\boldsymbol{\theta}, \boldsymbol{F}\nabla\boldsymbol{\theta}) - 2(L_{\boldsymbol{Fx}}\boldsymbol{\theta}, \boldsymbol{F}\nabla\boldsymbol{\theta}) + (L_{\boldsymbol{xx}}\boldsymbol{\theta}, \boldsymbol{\theta}). \tag{3.8}$$

3.2 Mixed inner-outer variations

With the new notation, introduced in Section 3.1, we can write the action of the inner-outer variation (2.6) on $I(\boldsymbol{y})$ as

$$I(\boldsymbol{y}_\epsilon) = I(\boldsymbol{y}(\boldsymbol{\vartheta}_\epsilon) + \epsilon\boldsymbol{\phi}(\boldsymbol{\vartheta}_\epsilon)) = \mathfrak{O}[\epsilon\boldsymbol{\phi}](\mathfrak{I}[\epsilon\boldsymbol{\theta}]I(\boldsymbol{y})). \tag{3.9}$$

From this we easily obtain the expression for the first and second variations, corresponding to (2.6).

Theorem **3.3.**

(a) For any $\boldsymbol{\phi} \in C^2(\overline{\Omega};\mathbb{R}^m)$ *and* $\boldsymbol{\theta} \in C^2(\overline{\Omega};\mathbb{R}^d)$

$$I(\boldsymbol{y}_\epsilon) = I(\boldsymbol{y}) + \epsilon\delta I(\boldsymbol{\phi},\boldsymbol{\theta}) + \frac{\epsilon^2}{2}\delta^2 I_\Omega(\boldsymbol{\phi},\boldsymbol{\theta}) + o(\epsilon^2), \tag{3.10}$$

where

$$\delta I_\Omega(\boldsymbol{\phi},\boldsymbol{\theta}) = (\Delta_o[\boldsymbol{\phi}] + \Delta_i[\boldsymbol{\theta}])I(\boldsymbol{y}) \tag{3.11}$$

and

$$\delta^2 I_\Omega(\boldsymbol{\phi},\boldsymbol{\theta}) = (\Delta_o[\boldsymbol{\phi}] + \Delta_i[\boldsymbol{\theta}])^2 I(\boldsymbol{y}) - \delta I_\Omega((\nabla\boldsymbol{\phi})\boldsymbol{\theta}, (\nabla\boldsymbol{\theta})\boldsymbol{\theta}) \tag{3.12}$$

(b) If $\boldsymbol{\phi} \in \mathrm{Var} \cap C^2(\overline{\Omega};\mathbb{R}^m)$, $\boldsymbol{\theta} \in C^2(\overline{\Omega};\mathbb{R}^d) \cap C_0(\Omega;\mathbb{R}^d)$ *and* $\delta I_\Omega(\boldsymbol{\phi},\boldsymbol{\theta}) = 0$ *for all* $\boldsymbol{\phi} \in \mathrm{Var}$ *and all* $\boldsymbol{\theta} \in C^1(\overline{\Omega};\mathbb{R}^d) \cap C_0(\Omega;\mathbb{R}^d)$, *then*

$$\Delta_i[\boldsymbol{\theta}]\Delta_o[\boldsymbol{\phi}]I(\boldsymbol{y}) = \Delta_o[\boldsymbol{\phi}]\Delta_i[\boldsymbol{\theta}]I(\boldsymbol{y}), \tag{3.13}$$

and

$$\delta^2 I_\Omega(\boldsymbol{\phi},\boldsymbol{\theta}) = (\Delta_o[\boldsymbol{\phi}] + \Delta_i[\boldsymbol{\theta}])^2 I(\boldsymbol{y}). \tag{3.14}$$

Proof. Expand (3.9) up to the second order in ϵ, using Lemmas 3.1 and 3.2.

$$I(\boldsymbol{y}_\epsilon) = \mathfrak{O}[\epsilon\boldsymbol{\phi}]\left\{I(\boldsymbol{y}) + \epsilon\Delta_i[\boldsymbol{\theta}]I(\boldsymbol{y}) + \frac{\epsilon^2}{2}(\Delta_i^2[\boldsymbol{\theta}] - \Delta_i[(\nabla\boldsymbol{\theta})\boldsymbol{\theta}])I(\boldsymbol{y})\right\} + o(\epsilon^2).$$

Observe that the operator $\mathfrak{O}[\epsilon\boldsymbol{\phi}]$ is linear. Therefore,

$$\begin{aligned}I(\boldsymbol{y}_\epsilon) = I(\boldsymbol{y}) &+ \epsilon\Delta_i[\boldsymbol{\theta}]I(\boldsymbol{y}) + \epsilon\Delta_o[\boldsymbol{\phi}]I(\boldsymbol{y}) \\ &+ \frac{\epsilon^2}{2}(\Delta_i^2[\boldsymbol{\theta}] - \Delta_i[(\nabla\boldsymbol{\theta})\boldsymbol{\theta}] + 2\Delta_o[\boldsymbol{\phi}](\Delta_i[\boldsymbol{\theta}]) + \Delta_o^2[\boldsymbol{\phi}])I(\boldsymbol{y}) + o(\epsilon^2).\end{aligned} \tag{3.15}$$

Formula (3.11) follows. To prove (3.13) we compute the commutator of $\Delta_i[\boldsymbol{\theta}]$ and $\Delta_o[\boldsymbol{\phi}]$ explicitly:

$$\begin{aligned}\delta_o[\boldsymbol{\phi}](\delta_i[\boldsymbol{\theta}]L) = (\boldsymbol{P}, \nabla\boldsymbol{\phi}((\nabla\cdot\boldsymbol{\theta})\boldsymbol{I} - \nabla\boldsymbol{\theta})) - (L_{\boldsymbol{FF}}\nabla\boldsymbol{\phi}, \boldsymbol{F}\nabla\boldsymbol{\theta}) + (L_{\boldsymbol{Fx}}\boldsymbol{\theta}, \nabla\boldsymbol{\phi}) \\ + (L_{\boldsymbol{y}}, \boldsymbol{\phi})\nabla\cdot\boldsymbol{\theta} - (L_{\boldsymbol{Fy}}\boldsymbol{\phi}, \boldsymbol{F}\nabla\boldsymbol{\theta}) + (L_{\boldsymbol{xy}}\boldsymbol{\phi}, \boldsymbol{\theta})\end{aligned} \tag{3.16}$$

and

$$\delta_i[\boldsymbol{\theta}](\delta_o[\boldsymbol{\phi}]L) = (\boldsymbol{P}, \nabla\cdot(\nabla\boldsymbol{\phi}\otimes\boldsymbol{\theta})) - (L_{\boldsymbol{FF}}\nabla\boldsymbol{\phi}, \boldsymbol{F}\nabla\boldsymbol{\theta}) + (L_{\boldsymbol{Fx}}\boldsymbol{\theta}, \nabla\boldsymbol{\phi}) \\ + (L_{\boldsymbol{y}}, \nabla\cdot(\boldsymbol{\phi}\otimes\boldsymbol{\theta})) - (L_{\boldsymbol{Fy}}\boldsymbol{\phi}, \boldsymbol{F}\nabla\boldsymbol{\theta}) + (L_{\boldsymbol{xy}}\boldsymbol{\phi}, \boldsymbol{\theta}). \quad (3.17)$$

Here

$$(\nabla\cdot(\nabla\boldsymbol{\phi}\otimes\boldsymbol{\theta}))_{i\alpha} = (\phi_{i,\alpha}\theta_\beta)_{,\beta}, \qquad (\nabla\cdot(\boldsymbol{\phi}\otimes\boldsymbol{\theta}))_i = (\phi_i\theta_\beta)_{,\beta}.$$

Therefore, we obtain

$$\Delta_i[\boldsymbol{\theta}]\Delta_o[\boldsymbol{\phi}] - \Delta_o[\boldsymbol{\phi}]\Delta_i[\boldsymbol{\theta}] = \Delta_o[(\nabla\boldsymbol{\phi})\boldsymbol{\theta}]. \quad (3.18)$$

Recalling that $\boldsymbol{\theta} = \boldsymbol{0}$ on $\partial\Omega$ we conclude that $(\nabla\boldsymbol{\phi})\boldsymbol{\theta} \in W_0^{1,\infty}(\Omega;\mathbb{R}^m) \subset \mathrm{Var}$. Hence (3.13) follows. Substituting (3.18) into (3.15) we obtain (3.12), since $(\nabla\boldsymbol{\theta})\boldsymbol{\theta} \in C^1(\overline{\Omega};\mathbb{R}^d)\cap C_0(\Omega;\mathbb{R}^d)$. Finally, applying (3.13) to (3.15) we obtain (3.14). □

In addition to the formula (3.12) for the second variation we will also need an explicit formula for $\delta^2 I_\Omega(\boldsymbol{\phi},\boldsymbol{\theta})$.

Theorem **3.4.**

$$\delta^2 I_\Omega(\boldsymbol{\phi},\boldsymbol{\theta}) = \int_\Omega \{2J_2(\nabla\boldsymbol{\theta})L + 2((L_{\boldsymbol{x}},\boldsymbol{\theta}) + (L_{\boldsymbol{y}},\boldsymbol{\phi}))\nabla\cdot\boldsymbol{\theta} + (L_{\boldsymbol{xx}}\boldsymbol{\theta},\boldsymbol{\theta}) + (L_{\boldsymbol{yy}}\boldsymbol{\phi},\boldsymbol{\phi}) + 2(L_{\boldsymbol{xy}}\boldsymbol{\phi},\boldsymbol{\theta}) \\ + 2(\boldsymbol{P}\Theta(\nabla\boldsymbol{\theta}),\boldsymbol{H}) + (L_{\boldsymbol{FF}}\boldsymbol{H},\boldsymbol{H}) + 2(L_{\boldsymbol{Fx}}\boldsymbol{\theta} + L_{\boldsymbol{Fy}}\boldsymbol{\phi},\boldsymbol{H})\}d\boldsymbol{x}, \quad (3.19)$$

where

$$\boldsymbol{H} = \nabla\boldsymbol{\phi} - \boldsymbol{F}\nabla\boldsymbol{\theta}, \qquad J_2(\boldsymbol{\xi}) = \frac{1}{2}((\mathrm{Tr}\,\boldsymbol{\xi})^2 - \mathrm{Tr}\,(\boldsymbol{\xi}^2)), \qquad \Theta(\boldsymbol{\xi}) = \nabla J_2(\boldsymbol{\xi}) = (\mathrm{Tr}\,\boldsymbol{\xi})\boldsymbol{I} - \boldsymbol{\xi}^T.$$

Proof. The result follows if we substitute formulas (3.4), (3.8), (3.16) and (3.17) into (3.12). □

4 Smooth extremals

At the first glance, mixed inner-outer variations (2.6) are considerably more general than the pure outer variations (2.4) and produce conditions $\delta I_\Omega(\boldsymbol{\phi},\boldsymbol{\theta}) = 0$ and $\delta^2 I_\Omega(\boldsymbol{\phi},\boldsymbol{\theta}) \ge 0$ that are stronger than the classical conditions $\delta I_\Omega(\boldsymbol{\phi},\boldsymbol{0}) = 0$ and $\delta^2 I_\Omega(\boldsymbol{\phi},\boldsymbol{0}) \ge 0$, that follow from stability with respect to the outer variations alone. However, when $\boldsymbol{y}(\boldsymbol{x})$ is of class C^1 the inner-outer variation (2.6) is equivalent to the pure outer variation (2.4). In other words, in the smooth case the weak variation of Lagrangian coordinates can always be represented as a weak variation of Eulerian coordinates. In what follows we shall refer to this situation as the Euler-Lagrange (EL) equivalence.

Remark 4.1. *The EL equivalence principle for smooth fields can be also used on any subset of Ω, that is free from singularities, even if $\boldsymbol{F}(\boldsymbol{x})$ has singularities elsewhere in Ω.*

4.1 EL equivalence as a variational symmetry

Let us recall the notion of variational symmetry [45] (see also [46]). Consider a family of weak perturbations of the graph $\Gamma_{\boldsymbol{y}}$:

$$\Gamma_{\boldsymbol{Y}_\epsilon} = \{(\boldsymbol{X}(\boldsymbol{x}, \boldsymbol{y}; \epsilon), \boldsymbol{Y}(\boldsymbol{x}, \boldsymbol{y}; \epsilon)) : (\boldsymbol{x}, \boldsymbol{y}) \in \Gamma_{\boldsymbol{y}}\}, \tag{4.1}$$

where the functions $\boldsymbol{X}$ and $\boldsymbol{Y}$ are smooth in all of their arguments and have the property $\boldsymbol{X}(\boldsymbol{x}, \boldsymbol{y}; 0) = \boldsymbol{x}$ and $\boldsymbol{Y}(\boldsymbol{x}, \boldsymbol{y}; 0) = \boldsymbol{y}$. When ϵ is small enough the set $\Gamma_{\boldsymbol{Y}_\epsilon}$ is still a graph of the function $\boldsymbol{Y}_\epsilon(\boldsymbol{X})$, $\boldsymbol{X} \in \Omega_\epsilon$, where $\Omega_\epsilon = \boldsymbol{X}(\Gamma_{\boldsymbol{y}}; \epsilon)$.

Definition 4.2. *The transformation*

$$\boldsymbol{X} = \boldsymbol{X}(\boldsymbol{x}, \boldsymbol{y}; \epsilon), \qquad \boldsymbol{Y} = \boldsymbol{Y}(\boldsymbol{x}, \boldsymbol{y}; \epsilon) \tag{4.2}$$

is called a variational symmetry *at $\boldsymbol{y}(\boldsymbol{x})$ if*

$$\int_{\Omega_\epsilon} L(\boldsymbol{X}, \boldsymbol{Y}_\epsilon(\boldsymbol{X}), \nabla_{\boldsymbol{X}} \boldsymbol{Y}_\epsilon(\boldsymbol{X})) d\boldsymbol{X} = \int_{\Omega} L(\boldsymbol{x}, \boldsymbol{y}(\boldsymbol{x}), \nabla \boldsymbol{y}(\boldsymbol{x})) d\boldsymbol{x}. \tag{4.3}$$

*holds **for all** smooth subsets Ω of $\mathbb{R}^d$.*

The existence of the variational symmetry is usually associated with some special properties of the Lagrangian. The Noether theorem [45] then states that there is a conservation law corresponding to each variational symmetry. In our case the Lagrangian has no assumed symmetries of this kind. The EL equivalence is a weaker *integral symmetry*, when the relation (4.3) holds only for the given domain Ω. To obtain the corresponding "conservation law", we differentiating (4.3) in ϵ at $\epsilon = 0$ to obtain

$$(\Delta_i[\boldsymbol{\theta}] + \Delta_o[\boldsymbol{\phi}]) I(\boldsymbol{y}) = 0 \tag{4.4}$$

at $\boldsymbol{y} = \boldsymbol{y}(\boldsymbol{x})$, where

$$\boldsymbol{\theta}(\boldsymbol{x}, \boldsymbol{y}) = \left.\frac{\partial \boldsymbol{X}(\boldsymbol{x}, \boldsymbol{y}; \epsilon)}{\partial \epsilon}\right|_{\epsilon=0}, \qquad \boldsymbol{\phi}(\boldsymbol{x}, \boldsymbol{y}) = \left.\frac{\partial \boldsymbol{Y}(\boldsymbol{x}, \boldsymbol{y}; \epsilon)}{\partial \epsilon}\right|_{\epsilon=0} \tag{4.5}$$

can be regarded as the infinitesimal generators of the integral symmetry. We emphasize that $\boldsymbol{y}(\boldsymbol{x})$ is not assumed to be an extremal, and the implication (4.3)⇒(4.4) holds for general Lipschitz maps $\boldsymbol{y}(\boldsymbol{x})$.

The EL equivalence principle, relating inner and outer variations for smooth maps $\boldsymbol{y}(\boldsymbol{x})$ can be restated as a possibility of making non-trivial inner and outer variations (4.2) whose effects cancel out producing no net change in the graph of $\boldsymbol{y}(\boldsymbol{x})$. This can be written in the form of an integral symmetry at $\boldsymbol{y}(\boldsymbol{x})$ with

$$\boldsymbol{X} = \Xi(\boldsymbol{x}, \boldsymbol{y}; \epsilon), \qquad \boldsymbol{Y} = \boldsymbol{y} + \boldsymbol{y}(\Xi(\boldsymbol{x}, \boldsymbol{y}; \epsilon)) - \boldsymbol{y}(\boldsymbol{x}), \tag{4.6}$$

where $\Xi(\boldsymbol{x},\boldsymbol{y};\epsilon)$ is an arbitrary smooth family of diffeomorphisms of $\Gamma_{\boldsymbol{y}}$ onto Ω. It is easy to verify that in this case the graph $\Gamma_{\boldsymbol{Y}_\epsilon}$, given by (4.1) coincides with the graph $\Gamma_{\boldsymbol{y}}$ of $\boldsymbol{y}(\boldsymbol{x})$. Hence, $\boldsymbol{Y}_\epsilon(\boldsymbol{X}) = \boldsymbol{y}(\boldsymbol{X})$ and the equality (4.3) holds. If the map $\boldsymbol{y}(\boldsymbol{x})$ is Lipschitz, then no weak outer transformation $\boldsymbol{Y}(\boldsymbol{x},\boldsymbol{y};\epsilon)$ in (4.1) can cancel out the effect of the weak inner transformation $\Xi(\boldsymbol{x},\boldsymbol{y};\epsilon)$. In fact, the function $\boldsymbol{y}(\Xi(\boldsymbol{x},\boldsymbol{y};\epsilon))$ will be non-differentiable in ϵ. It is in this sense that the smoothness of $\boldsymbol{y}(\boldsymbol{x})$ is required for the integral variational symmetry.

For smooth maps $\boldsymbol{y}(\boldsymbol{x})$ the infinitesimal generators (4.5) corresponding to (4.6) are

$$\left.\frac{\partial \Xi(\boldsymbol{x},\boldsymbol{y};\epsilon)}{\partial\epsilon}\right|_{\epsilon=0} = \boldsymbol{\eta}(\boldsymbol{x},\boldsymbol{y}), \qquad \left.\frac{\partial \boldsymbol{y}(\Xi(\boldsymbol{x},\boldsymbol{y};\epsilon))}{\partial\epsilon}\right|_{\epsilon=0} = \boldsymbol{F}(\boldsymbol{x})\boldsymbol{\eta}(\boldsymbol{x},\boldsymbol{y}).$$

The corresponding identity (4.4) then becomes

$$0 = (\Delta_i[\boldsymbol{\eta}] + \Delta_o[\boldsymbol{F}\boldsymbol{\eta}])I(\boldsymbol{y}) = \int_\Omega (\mathcal{E}^*(L) + \boldsymbol{F}^T\mathcal{E}(L), \boldsymbol{\eta})d\boldsymbol{x} + \int_{\partial\Omega} L(\boldsymbol{\eta},\boldsymbol{n})dS, \tag{4.7}$$

where

$$\mathcal{E}(L) = L_{\boldsymbol{y}} - \nabla\cdot\boldsymbol{P}, \qquad \mathcal{E}^*(L) = L_{\boldsymbol{x}} - \nabla\cdot\boldsymbol{P}^*. \tag{4.8}$$

The infinitesimal generator $\boldsymbol{\eta}$ can be chosen arbitrarily in $C_0^1(\Omega;\mathbb{R}^d)$, by taking $\Xi(\boldsymbol{x},\boldsymbol{y};\epsilon) = \boldsymbol{x} + \epsilon\boldsymbol{\eta}(\boldsymbol{x})$. Then, the integral relation (4.7) can be rewritten pointwise, giving the Noether's identity

$$L_{\boldsymbol{x}} - \nabla\cdot\boldsymbol{P}^* = -\boldsymbol{F}^T(L_{\boldsymbol{y}} - \nabla\cdot\boldsymbol{P}). \tag{4.9}$$

The surface integral in (4.7) vanishes since $(\boldsymbol{\eta},\boldsymbol{n}) = 0$, as a consequence of invariance of the domain Ω. Identity (4.9) implies that any C^2 extremal is stationary, i.e. $\mathcal{E}^*(L) = 0$. We can therefore interpret stationarity of smooth extremals as a manifestation of integral symmetry.

The "trivial" graph transformation (4.6) can also be combined with any other transformation (4.2) without changing its cumulative effect. This allows one to modify the generators $\boldsymbol{\theta}$ and $\boldsymbol{\phi}$ of the transformation (4.2) without changing what the transformation does to $\Gamma_{\boldsymbol{y}}$ in the first order of ϵ.

Our interest in second variation suggests that we should also consider the effect of the EL equivalence symmetry (4.6) on the second order generators

$$\boldsymbol{\theta}'(\boldsymbol{x},\boldsymbol{y}) = \left.\frac{\partial^2\boldsymbol{X}(\boldsymbol{x},\boldsymbol{y};\epsilon)}{\partial\epsilon^2}\right|_{\epsilon=0}, \qquad \boldsymbol{\phi}'(\boldsymbol{x},\boldsymbol{y}) = \left.\frac{\partial^2\boldsymbol{Y}(\boldsymbol{x},\boldsymbol{y};\epsilon)}{\partial\epsilon^2}\right|_{\epsilon=0}. \tag{4.10}$$

The second order generators of the trivial transformation (4.6) are $(\boldsymbol{\eta}',\boldsymbol{\rho}')$, where

$$\boldsymbol{\rho}' = (\nabla\boldsymbol{F}\boldsymbol{\eta})\boldsymbol{\eta} + \boldsymbol{F}\boldsymbol{\eta}'.$$

If we compose an arbitrary smooth transformation (4.2) with the trivial transformation (4.6), we will obtain the new transformation

$$\boldsymbol{X} = \boldsymbol{Z}(\boldsymbol{x},\boldsymbol{y};\epsilon), \qquad \boldsymbol{Y} = \boldsymbol{W}(\boldsymbol{x},\boldsymbol{y};\epsilon),$$

that is equivalent to the original one. However, its first and second order infinitesimal generators will differ from $(\boldsymbol{\theta}, \boldsymbol{\phi})$ and $(\boldsymbol{\theta}', \boldsymbol{\phi}')$. We compute

$$\left.\frac{\partial \boldsymbol{Z}(\boldsymbol{x}, \boldsymbol{y}; \epsilon)}{\partial \epsilon}\right|_{\epsilon=0} = \boldsymbol{\theta} + \boldsymbol{\eta}, \qquad \left.\frac{\partial \boldsymbol{W}(\boldsymbol{x}, \boldsymbol{y}; \epsilon)}{\partial \epsilon}\right|_{\epsilon=0} = \boldsymbol{\phi} + \boldsymbol{F}\boldsymbol{\eta}.$$

We conclude that the pairs of first order generators $(\boldsymbol{\theta}, \boldsymbol{\phi})$ and $(\boldsymbol{\theta}+\boldsymbol{\eta}, \boldsymbol{\phi}+\boldsymbol{F}\boldsymbol{\eta})$ are equivalent. Computing the second order infinitesimal generators of the combined transformation, we get

$$\begin{cases} \left.\dfrac{\partial^2 \boldsymbol{Z}(\boldsymbol{x}, \boldsymbol{y}; \epsilon)}{\partial \epsilon^2}\right|_{\epsilon=0} = \boldsymbol{\theta}' + \boldsymbol{\eta}' + 2\boldsymbol{\eta}_{\boldsymbol{x}}\boldsymbol{\theta} + 2\boldsymbol{\eta}_{\boldsymbol{y}}\boldsymbol{\phi}, \\ \\ \left.\dfrac{\partial^2 \boldsymbol{W}(\boldsymbol{x}, \boldsymbol{y}; \epsilon)}{\partial \epsilon^2}\right|_{\epsilon=0} = \boldsymbol{\phi}' + \boldsymbol{\rho}' + 2(\boldsymbol{\phi}_{\boldsymbol{x}} + \boldsymbol{\phi}_{\boldsymbol{y}}\boldsymbol{F})\boldsymbol{\eta} + 2\boldsymbol{F}(\boldsymbol{\eta}_{\boldsymbol{x}}\boldsymbol{\theta} - \boldsymbol{\theta}_{\boldsymbol{x}}\boldsymbol{\eta} + \boldsymbol{\eta}_{\boldsymbol{y}}\boldsymbol{\phi} - \boldsymbol{\theta}_{\boldsymbol{y}}\boldsymbol{F}\boldsymbol{\eta}). \end{cases}$$

We may use the freedom in the choice of generators $\boldsymbol{\eta}$ and $\boldsymbol{\eta}'$ in order to replace the original inner-outer variation with the pure outer variation (up to the second order in ϵ), if we choose

$$\boldsymbol{\eta} = -\boldsymbol{\theta}, \qquad \boldsymbol{\eta}' = -\boldsymbol{\theta}' + 2\boldsymbol{\theta}_{\boldsymbol{x}}\boldsymbol{\theta} + 2\boldsymbol{\theta}_{\boldsymbol{y}}\boldsymbol{\phi}.$$

Applying this principle to the variation (2.5) we obtain the equivalent outer variation

$$\boldsymbol{y} \mapsto \boldsymbol{y} + \epsilon\boldsymbol{\psi} + \frac{\epsilon^2}{2}\boldsymbol{\psi}' + o(\epsilon^2)$$

where $\boldsymbol{\psi}$ is given by (2.11) and

$$\boldsymbol{\psi}' = 2\boldsymbol{F}(\nabla\boldsymbol{\theta})\boldsymbol{\theta} - 2(\nabla\boldsymbol{\phi})\boldsymbol{\theta} + (\nabla\boldsymbol{F}\boldsymbol{\theta})\boldsymbol{\theta} = -2(\nabla\boldsymbol{\psi})\boldsymbol{\theta} - (\nabla\boldsymbol{F}\boldsymbol{\theta})\boldsymbol{\theta}. \tag{4.11}$$

One consequence of these calculations is the possibility to simplify the general expansion (3.10):

$$I(\boldsymbol{y}_\epsilon) = I(\boldsymbol{y}) + \epsilon\delta I_\Omega(\boldsymbol{\psi}, \mathbf{0}) + \frac{\epsilon^2}{2}(\delta I_\Omega(\boldsymbol{\psi}', \mathbf{0}) + \delta^2 I_\Omega(\boldsymbol{\psi}, \mathbf{0})). \tag{4.12}$$

In particular, when the first variation vanishes, we obtain

$$\delta^2 I_\Omega(\boldsymbol{\phi}, \boldsymbol{\theta}) = \delta^2 I_\Omega(\boldsymbol{\psi}, \mathbf{0}). \tag{4.13}$$

In conclusion we mention that the considerations of this section were limited to the case when the domain Ω was fixed by the transformations (4.2). In order to make the principle of EL equivalence applicable to variable domains we need to move beyond the present restricted definition of variational symmetry.

4.2 First variation for smooth extremals

In this section we assume that $\boldsymbol{y}(\boldsymbol{x})$ is of class C^2 on a subdomain D of Ω and is an extremal, i.e. satisfies the Euler-Lagrange equation

$$L_{\boldsymbol{y}} - \nabla \cdot \boldsymbol{P} = \boldsymbol{0}, \tag{4.14}$$

in the classical sense on D. The EL equivalence principle implies, via (4.9), that the stationarity condition

$$L_{\boldsymbol{x}} - \nabla \cdot \boldsymbol{P}^* = \boldsymbol{0}, \tag{4.15}$$

also known as the Eshelby equation in elasticity theory is satisfied, when $\boldsymbol{x} \in D$. Then the first variation on D can be expressed as a surface integral over ∂D.

THEOREM **4.3.** *Let $D \subset \Omega$ be a subdomain with Lipschitz boundary. Assume that $\boldsymbol{y} \in C^2(\overline{D}; \mathbb{R}^m)$ then*

$$\delta I_D(\boldsymbol{\phi}, \boldsymbol{\theta}) = \delta I_D(\boldsymbol{\psi}, \boldsymbol{0}) + \mathfrak{S}_1, \tag{4.16}$$

where δI_D is the first variation (3.11), in which Ω is replaced with D, and

$$\mathfrak{S}_1 = \int_{\partial D} L(\boldsymbol{\theta}, \boldsymbol{n}) dS.$$

In particular, when $\boldsymbol{y}(\boldsymbol{x})$ is an extremal on D

$$\delta I_D(\boldsymbol{\phi}, \boldsymbol{\theta}) = \int_{\partial D} \{(\boldsymbol{P}\boldsymbol{n}, \boldsymbol{\psi}) + L(\boldsymbol{\theta}, \boldsymbol{n})\} dS.$$

Proof. Substituting

$$\nabla \boldsymbol{\phi} = \nabla \boldsymbol{\psi} + \nabla \boldsymbol{F} \boldsymbol{\theta} + \boldsymbol{F} \nabla \boldsymbol{\theta}$$

into (3.11) we obtain

$$\delta I_D(\boldsymbol{\phi}, \boldsymbol{\theta}) = \int_D \{(L_{\boldsymbol{y}}, \boldsymbol{\psi}) + (\boldsymbol{P}, \nabla \boldsymbol{\psi}) + L \nabla \cdot \boldsymbol{\theta} + (L_{\boldsymbol{x}}, \boldsymbol{\theta}) + (L_{\boldsymbol{y}}, \boldsymbol{F}\boldsymbol{\theta}) + (\boldsymbol{P}, \boldsymbol{F} \nabla \boldsymbol{\theta})\} d\boldsymbol{x}.$$

Therefore,

$$\delta I_D(\boldsymbol{\phi}, \boldsymbol{\theta}) = \delta I_D(\boldsymbol{\psi}, \boldsymbol{0}) + \int_D \{L \nabla \cdot \boldsymbol{\theta} + (\nabla L, \boldsymbol{\theta})\} d\boldsymbol{x} = \delta I_D(\boldsymbol{\psi}, \boldsymbol{0}) + \int_D \nabla \cdot (L\boldsymbol{\theta}) d\boldsymbol{x}.$$

The result follows from the divergence theorem. □

Theorem 4.3 will be used in Section 5.1, where we derive the expression for the first variation $\delta I_\Omega(\boldsymbol{\phi}, \boldsymbol{\theta})$ for extremals with jump discontinuities.

4.3 Second variation for smooth extremals

The goal of this section is to prove the analog of Theorem 4.3 and formula (4.16) for second variation. The analysis here applies not only to the case when the extremal is smooth, but also to the case when it is piecewise smooth.

THEOREM **4.4.** *Let $D \subset \Omega$ be a subdomain with Lipschitz boundary. Assume $\boldsymbol{y} \in C^3(\overline{D};\mathbb{R}^m)$ is an extremal. Then*

$$\delta^2 I_D(\boldsymbol{\phi},\boldsymbol{\theta}) = \delta^2 I_D(\boldsymbol{\psi},\boldsymbol{0}) + \mathfrak{S}_2, \tag{4.17}$$

where

$$\mathfrak{S}_2 = \int_{\partial D}\{((\boldsymbol{P}^*)^T\nabla_{\partial D}\boldsymbol{\theta} + \boldsymbol{P}^T\nabla_{\partial D}(2\boldsymbol{\psi}+\boldsymbol{F}\boldsymbol{\theta}), (\boldsymbol{\theta},\boldsymbol{n})\boldsymbol{I} - \boldsymbol{n}\otimes\boldsymbol{\theta}) + ((L_{\boldsymbol{x}},\boldsymbol{\theta}) + (L_{\boldsymbol{y}}, 2\boldsymbol{\psi}+\boldsymbol{F}\boldsymbol{\theta}))(\boldsymbol{\theta},\boldsymbol{n})\}dS.$$

In particular, $\delta^2 I_D(\boldsymbol{\phi},\boldsymbol{\theta}) = \delta^2 I_D(\boldsymbol{\psi},\boldsymbol{0})$, when $\boldsymbol{\theta} = \boldsymbol{0}$ on ∂D. Here $\boldsymbol{\psi}(\boldsymbol{x})$ is given by (2.11) and

$$\nabla_{\partial D}\boldsymbol{f} = \nabla\boldsymbol{f} - \frac{\partial\boldsymbol{f}}{\partial\boldsymbol{n}}\otimes\boldsymbol{n} = \nabla\boldsymbol{f}(\boldsymbol{I}-\boldsymbol{n}\otimes\boldsymbol{n}) \tag{4.18}$$

is the surface gradient.

Proof. We begin by expressing $\boldsymbol{H}$ in (3.19) in terms of $\boldsymbol{\psi}$: $\boldsymbol{H} = \nabla\boldsymbol{\psi} + \nabla\boldsymbol{F}\boldsymbol{\theta}$. We then apply the chain rule identities

$$L_{\boldsymbol{F}\boldsymbol{F}}(\nabla\boldsymbol{F}\boldsymbol{\theta}) = \nabla\boldsymbol{P}\boldsymbol{\theta} - L_{\boldsymbol{F}\boldsymbol{x}}\boldsymbol{\theta} - L_{\boldsymbol{F}\boldsymbol{y}}(\boldsymbol{F}\boldsymbol{\theta})$$

$$L_{\boldsymbol{y}\boldsymbol{F}}(\nabla\boldsymbol{F}\boldsymbol{\theta}) = \nabla L_{\boldsymbol{y}}\boldsymbol{\theta} - L_{\boldsymbol{y}\boldsymbol{x}}\boldsymbol{\theta} - L_{\boldsymbol{y}\boldsymbol{y}}\boldsymbol{F}\boldsymbol{\theta}$$

$$(L_{\boldsymbol{x}\boldsymbol{F}}(\nabla\boldsymbol{F}\boldsymbol{\theta}),\boldsymbol{\theta}) = (\nabla L_{\boldsymbol{x}}\boldsymbol{\theta},\boldsymbol{\theta}) - (L_{\boldsymbol{x}\boldsymbol{x}}\boldsymbol{\theta},\boldsymbol{\theta}) - (L_{\boldsymbol{x}\boldsymbol{y}}\boldsymbol{F}\boldsymbol{\theta},\boldsymbol{\theta}).$$

We obtain

$$\delta^2 I_D(\boldsymbol{\phi},\boldsymbol{\theta}) = \delta^2 I_D(\boldsymbol{\psi},\boldsymbol{0}) + \int_D\{2J_2(\nabla\boldsymbol{\theta})L + 2((L_{\boldsymbol{x}},\boldsymbol{\theta}) + (L_{\boldsymbol{y}},\boldsymbol{\psi}+\boldsymbol{F}\boldsymbol{\theta}))\nabla\cdot\boldsymbol{\theta} + 2(\boldsymbol{P}\boldsymbol{\Theta},\nabla\boldsymbol{\psi}+\nabla\boldsymbol{F}\boldsymbol{\theta}) + 2(\nabla\boldsymbol{P}\boldsymbol{\theta},\nabla\boldsymbol{\psi}) + (\nabla\boldsymbol{P}\boldsymbol{\theta},\nabla\boldsymbol{F}\boldsymbol{\theta}) + (\nabla L_{\boldsymbol{y}}\boldsymbol{\theta},\boldsymbol{F}\boldsymbol{\theta}) + 2(\nabla L_{\boldsymbol{y}}\boldsymbol{\theta},\boldsymbol{\psi}) + (\nabla L_{\boldsymbol{x}}\boldsymbol{\theta},\boldsymbol{\theta})\}d\boldsymbol{x}.$$

We now show that the volume integral on the right-hand side above is equal to the surface integral in (4.17). To organize the calculations we split the integral above into 6 groups of terms and proceed to simplify and combine these groups until our goal is reached. We write

$$\delta^2 I_D(\boldsymbol{\phi},\boldsymbol{\theta}) = \delta^2 I_D(\boldsymbol{\psi},\boldsymbol{0}) + \sum_{j=1}^{6} T_j.$$

$$T_1 = \int_D\{2(\nabla\boldsymbol{P}\boldsymbol{\theta},\nabla\boldsymbol{\psi}) + (\nabla\boldsymbol{P}\boldsymbol{\theta},\nabla\boldsymbol{F}\boldsymbol{\theta}) + (\nabla L_{\boldsymbol{y}}\boldsymbol{\theta},\boldsymbol{F}\boldsymbol{\theta})\}d\boldsymbol{x}$$

$$T_2 = 2\int_D \{((L_{\boldsymbol{x}}, \boldsymbol{\theta}) + (L_{\boldsymbol{y}}, \boldsymbol{F\theta}))\nabla\cdot\boldsymbol{\theta} + (\boldsymbol{P\Theta}(\nabla\boldsymbol{\theta}), \nabla\boldsymbol{F\theta})\}d\boldsymbol{x}$$

$$T_3 = 2\int_D (\boldsymbol{P\Theta}(\nabla\boldsymbol{\theta}), \nabla\boldsymbol{\psi})d\boldsymbol{x}, \qquad T_4 = 2\int_D \{(L_{\boldsymbol{y}}, \boldsymbol{\psi})\nabla\cdot\boldsymbol{\theta} + (\nabla L_{\boldsymbol{y}}\boldsymbol{\theta}, \boldsymbol{\psi})\}d\boldsymbol{x}$$

$$T_5 = 2\int_D J_2(\nabla\boldsymbol{\theta})L d\boldsymbol{x}, \qquad T_6 = \int_D (\nabla L_{\boldsymbol{x}}\boldsymbol{\theta}, \boldsymbol{\theta})d\boldsymbol{x}$$

Step 1. We integrate by parts in the first and second terms of T_1, using (4.14) in the second term:

$$T_1 = Y_1 + X_1 + S_1 + S_2$$

where

$$Y_1 = -2\int_D (\boldsymbol{P}, \nabla\nabla\boldsymbol{\psi\theta} + \nabla\boldsymbol{\psi}\nabla\cdot\boldsymbol{\theta})d\boldsymbol{x}, \quad X_1 = -\int_D P_{i\alpha,\beta}F_{i\gamma}(\theta_\beta\theta_\gamma)_{,\alpha}d\boldsymbol{x},$$

$$S_1 = 2\int_{\partial D} (\boldsymbol{P}, \nabla\boldsymbol{\psi})(\boldsymbol{\theta}, \boldsymbol{n})dS, \qquad S_2 = \int_{\partial D} ((\nabla\boldsymbol{P\theta})\boldsymbol{n}, \boldsymbol{F\theta})dS$$

Hence, we obtain

$$\delta^2 I_D(\boldsymbol{\phi}, \boldsymbol{\theta}) = \delta^2 I_D(\boldsymbol{\psi}, \boldsymbol{0}) + X_1 + Y_1 + S_1 + S_2 + T_2 + T_3 + T_4 + T_5 + T_6.$$

Step 2. $T_2 = X_2 + X_3$, where

$$X_2 = 2\int_D (\nabla L, \boldsymbol{\theta})\nabla\cdot\boldsymbol{\theta}d\boldsymbol{x}, \qquad X_3 = -2\int_D (\nabla\boldsymbol{F\theta}, \boldsymbol{P}(\nabla\boldsymbol{\theta})^T)d\boldsymbol{x}.$$

We also observe that

$$X_1 + X_3 = X_4 = -\int_D (F_{i\gamma}P_{i\alpha})_{,\beta}(\theta_\beta\theta_\gamma)_{,\alpha}d\boldsymbol{x}.$$

Hence,

$$\delta^2 I_D(\boldsymbol{\phi}, \boldsymbol{\theta}) = \delta^2 I_D(\boldsymbol{\psi}, \boldsymbol{0}) + X_2 + X_4 + Y_1 + S_1 + S_2 + T_3 + T_4 + T_5 + T_6.$$

Step 3. We integrate by parts and use (4.14).

$$Y_1 + T_3 = -2\int_D (\boldsymbol{P}, \nabla(\nabla\boldsymbol{\psi\theta}))d\boldsymbol{x} = Y_2 + S_3,$$

where

$$Y_2 = 2\int_D (L_{\boldsymbol{y}}, \nabla\boldsymbol{\psi\theta})d\boldsymbol{x}, \qquad S_3 = -2\int_{\partial D} (\boldsymbol{Pn}, \nabla\boldsymbol{\psi\theta})dS.$$

We also have

$$S_1 + S_3 = Z_1 = 2\int_{\partial D} (\nabla_{\partial D}\boldsymbol{\psi}, \boldsymbol{P}((\boldsymbol{\theta}, \boldsymbol{n})\boldsymbol{I} - \boldsymbol{n}\otimes\boldsymbol{\theta}))dS.$$

Hence,
$$\delta^2 I_D(\boldsymbol{\phi},\boldsymbol{\theta}) = \delta^2 I_D(\boldsymbol{\psi},\mathbf{0}) + X_2 + X_4 + Y_2 + Z_1 + S_2 + T_4 + T_5 + T_6.$$

Step 4.
$$Y_2 + T_4 = 2\int_D \nabla\cdot((L_{\boldsymbol{y}},\boldsymbol{\psi})\boldsymbol{\theta})d\boldsymbol{x} = S_4,$$
where
$$S_4 = 2\int_{\partial D}(L_{\boldsymbol{y}},\boldsymbol{\psi})(\boldsymbol{\theta},\boldsymbol{n})dS.$$
Hence,
$$\delta^2 I_D(\boldsymbol{\phi},\boldsymbol{\theta}) = \delta^2 I_D(\boldsymbol{\psi},\mathbf{0}) + X_2 + X_4 + Z_1 + S_2 + S_4 + T_5 + T_6.$$

Step 5. We represent $J_2(\nabla\boldsymbol{\theta})$ as a divergence, $2J_2(\nabla\boldsymbol{\theta}) = \nabla\cdot(\boldsymbol{\Theta}^T(\nabla\boldsymbol{\theta})\boldsymbol{\theta})$, and integrate by parts
$$T_5 = S_5 + X_5,$$
where
$$X_5 = -\int_D(\nabla L,\boldsymbol{\Theta}^T(\nabla\boldsymbol{\theta})\boldsymbol{\theta})d\boldsymbol{x},\qquad S_5 = \int_{\partial D}(\boldsymbol{\theta},\boldsymbol{\Theta}(\nabla\boldsymbol{\theta})\boldsymbol{n})LdS.$$
We compute
$$X_5 + X_2 = X_6 = \int_D L_{,\beta}(\theta_\alpha\theta_\beta)_{,\alpha}d\boldsymbol{x} = \int_D (L\delta_{\gamma\alpha})_{,\beta}(\theta_\beta\theta_\gamma)_{,\alpha}d\boldsymbol{x}$$
Observe that
$$X_4 + X_6 = \int_D\{(L\delta_{\gamma\alpha})_{,\beta}(\theta_\beta\theta_\gamma)_{,\alpha} - (F_{i\gamma}P_{i\alpha})_{,\beta}(\theta_\beta\theta_\gamma)_{,\alpha}\}d\boldsymbol{x} = \int_D P^*_{\gamma\alpha,\beta}(\theta_\beta\theta_\gamma)_{,\alpha}d\boldsymbol{x}.$$
Then, integrating by parts and using (4.15), we obtain $X_4 + X_6 = X_7 + S_6$, where
$$X_7 = -\int_D(\nabla L_{\boldsymbol{x}}\boldsymbol{\theta},\boldsymbol{\theta})d\boldsymbol{x},\qquad S_6 = \int_{\partial D}((\nabla\boldsymbol{P}^*\boldsymbol{\theta})\boldsymbol{n},\boldsymbol{\theta})dS.$$
We have
$$\nabla\boldsymbol{P}^*\boldsymbol{\theta} = (L_{\boldsymbol{x}},\boldsymbol{\theta})\boldsymbol{I} + (L_{\boldsymbol{y}},\boldsymbol{F}\boldsymbol{\theta})\boldsymbol{I} + (\boldsymbol{P},\nabla\boldsymbol{F}\boldsymbol{\theta})\boldsymbol{I} - (\nabla\boldsymbol{F}\boldsymbol{\theta})^T\boldsymbol{P} - \boldsymbol{F}^T\nabla\boldsymbol{P}\boldsymbol{\theta}.$$
Therefore, $S_2 + S_6 = S_7 + S_8$, where
$$S_7 = \int_{\partial D}\{(L_{\boldsymbol{x}},\boldsymbol{\theta})(\boldsymbol{\theta},\boldsymbol{n}) + (L_{\boldsymbol{y}},\boldsymbol{F}\boldsymbol{\theta})(\boldsymbol{\theta},\boldsymbol{n})\}dS.$$
and
$$S_8 = \int_{\partial D}(\nabla\boldsymbol{F}\boldsymbol{\theta},\boldsymbol{P}((\boldsymbol{\theta},\boldsymbol{n})\boldsymbol{I} - \boldsymbol{n}\otimes\boldsymbol{\theta}))dS,$$

Next, observe that

$$\nabla \boldsymbol{F}\boldsymbol{\theta} = \nabla_{\partial D}(\boldsymbol{F}\boldsymbol{\theta}) - \boldsymbol{F}\nabla_{\partial D}\boldsymbol{\theta} + \frac{\partial \boldsymbol{F}}{\partial \boldsymbol{n}}\boldsymbol{\theta} \otimes \boldsymbol{n}.$$

Therefore,

$$S_8 = \int_{\partial D} (\nabla_{\partial D}(\boldsymbol{F}\boldsymbol{\theta}) - \boldsymbol{F}\nabla_{\partial D}\boldsymbol{\theta}, \boldsymbol{P}((\boldsymbol{\theta}, \boldsymbol{n})\boldsymbol{I} - \boldsymbol{n} \otimes \boldsymbol{\theta}))dS.$$

We also have

$$(\boldsymbol{\Theta}^T(\nabla\boldsymbol{\theta})\boldsymbol{\theta}, \boldsymbol{n}) = (\nabla \cdot \boldsymbol{\theta})(\boldsymbol{\theta}, \boldsymbol{n}) - ((\nabla\boldsymbol{\theta})\boldsymbol{\theta}, \boldsymbol{n}) = (\nabla_{\partial D}\boldsymbol{\theta}, (\boldsymbol{\theta}, \boldsymbol{n})\boldsymbol{I} - \boldsymbol{n} \otimes \boldsymbol{\theta}).$$

Hence, $S_2 + S_5 + S_6 = S_7 + Z_2$, where

$$Z_2 = \int_{\partial D} (\boldsymbol{P}^T\nabla_{\partial D}(\boldsymbol{F}\boldsymbol{\theta}) + (\boldsymbol{P}^*)^T\nabla_{\partial D}\boldsymbol{\theta}, (\boldsymbol{\theta}, \boldsymbol{n})\boldsymbol{I} - \boldsymbol{n} \otimes \boldsymbol{\theta})\}dS.$$

Step 6. Finally, observe that $X_7 + T_6 = 0$. Hence,

$$\delta^2 I_D(\boldsymbol{\phi}, \boldsymbol{\theta}) = \delta^2 I_D(\boldsymbol{\psi}, \boldsymbol{0}) + Z_1 + Z_2 + S_4 + S_7.$$

When $\boldsymbol{\theta}(\boldsymbol{x}) = \boldsymbol{0}$ on ∂D, all surface integrals Z_1, Z_2, S_4 and S_7 vanish. The theorem is proved. □

Remark 4.5. *If we do not assume that $\boldsymbol{y}(\boldsymbol{x})$ is an extremal in Theorem 4.4, then*

$$\delta^2 I_D(\boldsymbol{\phi}, \boldsymbol{\theta}) = \delta^2 I_D(\boldsymbol{\psi}, \boldsymbol{0}) + \mathfrak{S}_2 + \int_D (\mathcal{E}(L), \boldsymbol{\psi}')d\boldsymbol{x}, \tag{4.19}$$

where $\mathcal{E}(L)$ and $\boldsymbol{\psi}'$ are given by (4.8) and (4.11), respectively. It follows that Theorem 4.4 is valid for $\boldsymbol{y} \in C^2(\overline{\Omega}; \mathbb{R}^d)$. Indeed, let $\boldsymbol{y}_n \in C^3(\overline{\Omega}; \mathbb{R}^d)$ be such that $\boldsymbol{y}_n \to \boldsymbol{y}$ in $C^2(\overline{\Omega}; \mathbb{R}^d)$, as $n \to \infty$. Passing to the limit, we conclude that (4.19) holds for $\boldsymbol{y} \in C^2(\overline{\Omega}; \mathbb{R}^d)$, since both sides of (4.19) involve derivatives of $\boldsymbol{y}(\boldsymbol{x})$ only up to order 2. The formula (4.17) follows, if $\boldsymbol{y}(\boldsymbol{x})$ is an extremal.

5 Extremals with jump discontinuities

In this section we focus on the case when $\boldsymbol{F}(\boldsymbol{x})$ has a jump discontinuity across a smooth interface Σ. We will derive the formulas for the first and second variation corresponding to inner-outer variation (2.6) in two ways. One, using the partial EL equivalence principle only on the smooth part of Ω via Theorems 4.3 and 4.4. The other, using the full EL equivalence principle extended to strong variations and studying $\Delta I(\boldsymbol{\phi}_\epsilon)$ for the EL equivalent variation (2.8).

Suppose that we can split Ω into the disjoint union of two domains Ω_+, Ω_- (i.e. $\overline{\Omega} = \overline{\Omega_+} \cup \overline{\Omega_-}$, $\overline{\Omega_+} \cap \overline{\Omega_-} = \emptyset$), such that $\boldsymbol{y}(\boldsymbol{x})$ is of class C^2 on both $\overline{\Omega_+}$ and $\overline{\Omega_-}$. We assume that $\nabla\boldsymbol{y}(\boldsymbol{x})$ has a jump discontinuity across a smooth surface $\Sigma \subset \overline{\Omega_+} \cap \overline{\Omega_-}$. By our convention the unit normal on Σ always points from Ω_- into Ω_+.

5.1 First variation via partial EL equivalence

If $\boldsymbol{y}(\boldsymbol{x})$ satisfies conditions of equilibrium in the bulk, then the first variation reduces to the the integral over the surface of discontinuity Σ. The vanishing of that integral results in the conditions of equilibrium for the surface Σ in the Eulerian and Lagrangian coordinates.

THEOREM **5.1.** *Assume that the Lipschitz map $\boldsymbol{y} : \Omega \to \mathbb{R}^m$ is of class C^2 on $\overline{\Omega_\pm}$ and satisfies the Euler-Lagrange equation (4.14) on $\Omega_\pm$. Then*

$$\delta I_\Omega(\boldsymbol{\phi}, \boldsymbol{\theta}) = -\int_\Sigma \{([\![\boldsymbol{P}]\!]\boldsymbol{n}, \{\!\!\{\boldsymbol{\psi}\}\!\!\}) + p^*\xi(\boldsymbol{x})\} dS, \tag{5.1}$$

where $\xi(\boldsymbol{x}) = (\boldsymbol{\theta}, \boldsymbol{n})$ and

$$p^* = [\![L]\!] - (\{\!\!\{\boldsymbol{P}\}\!\!\}, [\![\boldsymbol{F}]\!]) \tag{5.2}$$

is called the Maxwell driving force on Σ. Here $\{\!\!\{a\}\!\!\} = \frac{1}{2}(a_+ + a_-)$ and $[\![a]\!] = a_+ - a_-$.

Proof. According to Theorem 4.3

$$\delta I_\Omega(\boldsymbol{\phi}, \boldsymbol{\theta}) = \delta I_{\Omega_+}(\boldsymbol{\psi}, \boldsymbol{0}) + \delta I_{\Omega_-}(\boldsymbol{\psi}, \boldsymbol{0}) - \int_\Sigma [\![L]\!](\boldsymbol{\theta}, \boldsymbol{n}) dS. \tag{5.3}$$

Integrating by parts and using the Euler-Lagrange equation (4.14) on $\Omega_\pm$ we obtain

$$\delta I_\Omega(\boldsymbol{\phi}, \boldsymbol{\theta}) = -\int_\Sigma \{[\![(\boldsymbol{P}\boldsymbol{n}, \boldsymbol{\psi})]\!] + [\![L]\!](\boldsymbol{\theta}, \boldsymbol{n})\} dS.$$

We note that according to (2.11), $\boldsymbol{\psi}(\boldsymbol{x})$ has a jump discontinuity across Σ:

$$[\![\boldsymbol{\psi}]\!] = -[\![\boldsymbol{F}]\!]\boldsymbol{\theta}. \tag{5.4}$$

Using (5.4) and the product rule

$$[\![ab]\!] = [\![a]\!]\{\!\!\{b\}\!\!\} + \{\!\!\{a\}\!\!\}[\![b]\!] \tag{5.5}$$

we obtain

$$\delta I_\Omega(\boldsymbol{\phi}, \boldsymbol{\theta}) = -\int_\Sigma \{([\![\boldsymbol{P}]\!]\boldsymbol{n}, \{\!\!\{\boldsymbol{\psi}\}\!\!\}) - (\{\!\!\{\boldsymbol{P}\}\!\!\}\boldsymbol{n}, [\![\boldsymbol{F}]\!]\boldsymbol{\theta}) + [\![L]\!](\boldsymbol{\theta}, \boldsymbol{n})\} dS.$$

Now we take into account the continuity of $\boldsymbol{y}$ across the interface Σ in the form of the kinematic compatibility relation of Hadamard

$$[\![\boldsymbol{F}]\!] = \boldsymbol{a} \otimes \boldsymbol{n}, \tag{5.6}$$

where $\boldsymbol{a}\colon \Sigma \to \mathbb{R}^m$. Recalling the definition (5.2) of p^*, we obtain (5.1). □

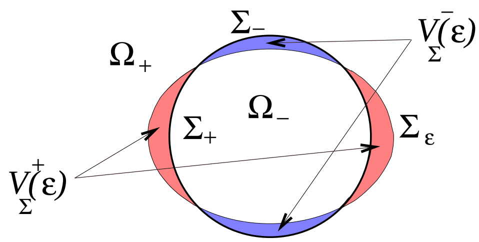

Figure 2: Regions $V_\Sigma^{\pm}(\epsilon)$.

Since the fields $\{\boldsymbol{\psi}\}$ and ξ can be chosen arbitrarily and independently on Σ, the vanishing of the first variation implies the condition of equilibrium of Σ in Eulerian coordinates:

$$[\![\boldsymbol{P}]\!]\boldsymbol{n} = \boldsymbol{0}, \tag{5.7}$$

as well as the condition of equilibrium of Σ in Lagrangian coordinates:

$$p^* = 0. \tag{5.8}$$

We have obtained $m+1$ interface conditions (5.7–5.8), even though we have started with $m+d$ independent variations $\boldsymbol{\phi}$ and $\boldsymbol{\theta}$. This is explained by the principle of EL equivalence, according to which the variation fields $\boldsymbol{\phi}$ and $\boldsymbol{\theta}$ enter the first variation δI_Ω through the total discontinuous variation $\boldsymbol{\psi}$. The formula (5.4) combined with (5.6) implies that

$$[\![\boldsymbol{\psi}]\!] = -\boldsymbol{a}(\boldsymbol{\theta}, \boldsymbol{n}) = -\xi(\boldsymbol{x})[\![\boldsymbol{F}]\!]\boldsymbol{n}, \qquad \xi(\boldsymbol{x}) = (\boldsymbol{\theta}, \boldsymbol{n}). \tag{5.9}$$

Hence the variations $\boldsymbol{\theta}$ and $\boldsymbol{\phi}$ enter the variation δI_Ω through m independent field variations $\{\boldsymbol{\psi}\}$ and a single scalar surface variation field $\xi(\boldsymbol{x})$. The new degree of freedom ξ comes from the necessity to locate the surface of discontinuity in the d-dimensional space of Lagrangian labels.

5.2 First variation via full EL equivalence

The formula (5.1) can also be derived directly, by investigating the structure of the equivalent strong outer variation $\boldsymbol{\phi}_\epsilon(\boldsymbol{x})$, given by (2.8). Observe that the Taylor expansion (2.10) is still valid for all $\boldsymbol{x}$ away from a small neighborhood of Σ. Therefore, one can use the equivalent variation $\boldsymbol{\phi}_\epsilon(\boldsymbol{x}) \sim \epsilon\boldsymbol{\psi}$, given by (2.11), on most of the domain Ω. The Taylor expansion (2.10) breaks down only in the small set $V_\Sigma(\epsilon)$ containing Σ (see Figure 2)

$$V_\Sigma^{\pm}(\epsilon) = \{\boldsymbol{x} \in \Omega_\pm : \boldsymbol{\vartheta}_\epsilon(\boldsymbol{x}) \in \Omega_\mp\}. \tag{5.10}$$

We denote $V_\Sigma(\epsilon) = V_\Sigma^+(\epsilon) \cup V_\Sigma^-(\epsilon)$ and observe that the estimate (2.10) remains uniform in $\boldsymbol{x} \in \Omega \setminus V_\Sigma(\epsilon)$.

For $\boldsymbol{x} \in V_\Sigma(\epsilon)$ it will be convenient to use the curvilinear orthogonal coordinate system based on Σ. Let $\boldsymbol{x} = \boldsymbol{p}(\boldsymbol{u})$, $\boldsymbol{u} \in U \subset \mathbb{R}^{d-1}$ be a local parametrization of Σ. When ϵ is small enough, every $\boldsymbol{x} \in V_\Sigma(\epsilon)$ has a unique representation

$$\boldsymbol{x} = \boldsymbol{p}(\boldsymbol{u}) + z\boldsymbol{n}(\boldsymbol{u}), \tag{5.11}$$

where $\boldsymbol{n}(\boldsymbol{u})$ is the unit normal to Σ at $\boldsymbol{x} = \boldsymbol{p}(\boldsymbol{u})$, pointing from Ω_- into Ω_+. The standard Taylor expansion yields

$$\boldsymbol{\vartheta}_\epsilon(\boldsymbol{x}) = \boldsymbol{p}(\boldsymbol{u}) + z\boldsymbol{n}(\boldsymbol{u}) - \epsilon\boldsymbol{\theta}(\boldsymbol{u}) + O(\epsilon^2), \tag{5.12}$$

where $\boldsymbol{\theta}(\boldsymbol{u})$ is a shorthand for $\boldsymbol{\theta}(\boldsymbol{p}(\boldsymbol{u}))$. If $\boldsymbol{x} \in V_\Sigma^+(\epsilon)$ then $0 < z < \zeta(\boldsymbol{u};\epsilon)$, while, if $\boldsymbol{x} \in V_\Sigma^-(\epsilon)$ then $0 > z > \zeta(\boldsymbol{u};\epsilon)$, where

$$\zeta(\boldsymbol{u};\epsilon) = \epsilon\xi(\boldsymbol{u}) + O(\epsilon^2), \qquad \xi(\boldsymbol{u}) = (\boldsymbol{\theta}(\boldsymbol{u}), \boldsymbol{n}). \tag{5.13}$$

In particular, $z = O(\epsilon)$. We are now ready to analyze the equivalent outer variation.

We handle the jump discontinuity of $\boldsymbol{F}(\boldsymbol{x})$ by using the Taylor expansion around $\boldsymbol{p}(\boldsymbol{u})$, instead of the Taylor expansion (2.10) around $\boldsymbol{x}$. We write

$$\boldsymbol{F}_\epsilon(\boldsymbol{x}) = \boldsymbol{F}(\boldsymbol{\vartheta}_\epsilon(\boldsymbol{x}))\nabla\boldsymbol{\vartheta}_\epsilon(\boldsymbol{x}) + \epsilon\nabla\boldsymbol{\phi}(\boldsymbol{\vartheta}_\epsilon(\boldsymbol{x}))\nabla\boldsymbol{\vartheta}_\epsilon(\boldsymbol{x}),$$

where $\boldsymbol{\vartheta}_\epsilon(\boldsymbol{x})$ is given by (5.12) and

$$\nabla\boldsymbol{\vartheta}_\epsilon(\boldsymbol{x}) = (\boldsymbol{I} + \epsilon\nabla\boldsymbol{\theta}(\boldsymbol{x}) + O(\epsilon^2))^{-1} = \boldsymbol{I} - \epsilon(\nabla_{\boldsymbol{x}}\boldsymbol{\theta})(\boldsymbol{u}) + O(\epsilon^2).$$

Using these formulas to expand $\boldsymbol{F}_\epsilon(\boldsymbol{x})$, we obtain for $\boldsymbol{x} \in V_\Sigma^\pm(\epsilon)$

$$\boldsymbol{F}_\epsilon(\boldsymbol{x}) = \boldsymbol{F}_\mp + z\frac{\partial\boldsymbol{F}_\mp}{\partial\boldsymbol{n}} + \epsilon\nabla\boldsymbol{\psi}_\mp + o(\epsilon),$$

where $\boldsymbol{\psi}$ is the equivalent weak outer variation away from Σ, given by (2.11). Also,

$$\boldsymbol{F}(\boldsymbol{x}) = \boldsymbol{F}_\pm + z\frac{\partial\boldsymbol{F}_\pm}{\partial\boldsymbol{n}} + o(\epsilon).$$

The gradient of the equivalent outer variation is then equal to

$$\nabla\boldsymbol{\phi}_\epsilon = \boldsymbol{F}_\epsilon(\boldsymbol{x}) - \boldsymbol{F}(\boldsymbol{x}) = \begin{cases} \mp[\![\boldsymbol{F}]\!] \mp z[\![\dfrac{\partial\boldsymbol{F}}{\partial\boldsymbol{n}}]\!] + \epsilon\nabla\boldsymbol{\psi}_\mp + o(\epsilon), & \boldsymbol{x} \in V_\Sigma^\pm(\epsilon), \\ \epsilon\nabla\boldsymbol{\psi}(\boldsymbol{x}) + o(\epsilon), & \boldsymbol{x} \notin V_\Sigma(\epsilon). \end{cases} \tag{5.14}$$

We may now apply the same Taylor expansion to $\boldsymbol{y}_\epsilon(\boldsymbol{x})$ and $\boldsymbol{y}(\boldsymbol{x})$ as we have already done for $\boldsymbol{F}_\epsilon(\boldsymbol{x})$ and $\boldsymbol{F}(\boldsymbol{x})$. We then obtain the structure of the equivalent outer variation $\boldsymbol{\phi}_\epsilon = \boldsymbol{y}_\epsilon(\boldsymbol{x}) - \boldsymbol{y}(\boldsymbol{x})$,

$$\boldsymbol{\phi}_\epsilon = \begin{cases} \epsilon\boldsymbol{\phi}_0^\pm\left(\boldsymbol{u}, \dfrac{z}{\epsilon}\right) + o(\epsilon), & \boldsymbol{x} \in V_\Sigma^\pm(\epsilon) \\ \epsilon\boldsymbol{\psi}(\boldsymbol{x}) + o(\epsilon), & \boldsymbol{x} \notin V_\Sigma(\epsilon), \end{cases} \tag{5.15}$$

where

$$\boldsymbol{\phi}_0^\pm(\boldsymbol{u},\tau) = \boldsymbol{\psi}_\mp \mp \tau[\![\boldsymbol{F}]\!]\boldsymbol{n}.$$

One can see that the equivalent outer variation is not a weak variation. It is localized in the normal direction around the surface Σ, while it has the form (2.4) of the weak variation outside of $V_\Sigma(\epsilon)$. In physical terms this variation can be associated with the nucleation of a new phase at the surface of discontinuity. The nucleation is very special because it can also be regarded as a displacement of the phase boundary in Lagrangian coordinates.

Observe that the EL equivalent variation gradient $\nabla\boldsymbol{\phi}_\epsilon$ is not small on a small set $V_\Sigma(\epsilon)$, while it is small on a large set $\Omega\setminus V_\Sigma(\epsilon)$. In such situations one can use the Taylor expansion combined with the Euler-Lagrange equations. We start with

$$I(\boldsymbol{y}_\epsilon)-I(\boldsymbol{y})=\int_{\Omega_+}L^\star d\boldsymbol{x}+\int_{\Omega_-}L^\star d\boldsymbol{x}-\int_\Sigma[\![(\boldsymbol{P}\boldsymbol{n},\boldsymbol{\phi}_\epsilon)]\!]dS,$$

where

$$L^\star=L(\boldsymbol{x},\boldsymbol{y}(\boldsymbol{x})+\boldsymbol{\phi}_\epsilon,\nabla\boldsymbol{y}+\nabla\boldsymbol{\phi}_\epsilon)-L(\boldsymbol{x})-(L_{\boldsymbol{y}}(\boldsymbol{x}),\boldsymbol{\phi}_\epsilon)-(\boldsymbol{P}(\boldsymbol{x}),\nabla\boldsymbol{\phi}_\epsilon),$$

and $L(\boldsymbol{x})$, $L_{\boldsymbol{y}}(\boldsymbol{x})$ and $\boldsymbol{P}(\boldsymbol{x})$ denote L, $L_{\boldsymbol{y}}$ and $L_{\boldsymbol{F}}$, respectively, evaluated at $(\boldsymbol{x},\boldsymbol{y}(\boldsymbol{x}),\nabla\boldsymbol{y}(\boldsymbol{x}))$. Obviously, $L^\star=O(\epsilon^2)$ on $\Omega\setminus V_\Sigma(\epsilon)$. Therefore,

$$I(\boldsymbol{y}_\epsilon)-I(\boldsymbol{y})=\int_{V_\Sigma^+(\epsilon)}L^\star d\boldsymbol{x}+\int_{V_\Sigma^+(\epsilon)}L^\star d\boldsymbol{x}-\int_\Sigma([\![\boldsymbol{P}]\!]\boldsymbol{n},\boldsymbol{\phi}_\epsilon)dS+O(\epsilon^2).$$

Also, due to (5.13)

$$\int_{V_\Sigma^\pm(\epsilon)}L^\star d\boldsymbol{x}=\pm\int_{\Sigma_\pm}\int_0^{\epsilon\xi}L^\star dz dS(\boldsymbol{u})+O(\epsilon^2),$$

where $\Sigma_\pm=\Sigma\cap\overline{V_\Sigma^\pm(\epsilon)}$. When $\boldsymbol{x}\in V_\Sigma^\pm(\epsilon)$ we have $L^\star=\mp[\![L]\!]\pm(\boldsymbol{P}_\pm,[\![\boldsymbol{F}]\!])+O(\epsilon)$, while $\boldsymbol{\phi}_\epsilon=\epsilon\boldsymbol{\psi}_\mp+o(\epsilon)$, when $\boldsymbol{x}\in\Sigma_\pm$. Therefore, expressing

$$\boldsymbol{P}_\pm=\{\!\!\{\boldsymbol{P}\}\!\!\}\pm\frac{1}{2}[\![\boldsymbol{P}]\!],\qquad \boldsymbol{\psi}_\pm=\{\!\!\{\boldsymbol{\psi}\}\!\!\}\mp\frac{1}{2}\boldsymbol{a}(\boldsymbol{u})\xi(\boldsymbol{u}),$$

we obtain

$$\delta I_\Omega(\boldsymbol{\phi},\boldsymbol{\theta})=\lim_{\epsilon\to0}\frac{I(\boldsymbol{y}+\boldsymbol{\phi}_\epsilon)-I(\boldsymbol{y})}{\epsilon}=-\int_\Sigma\{([\![\boldsymbol{P}]\!]\boldsymbol{n},\{\!\!\{\boldsymbol{\psi}\}\!\!\})+p^*\xi(\boldsymbol{u})\}dS(\boldsymbol{u}),$$

thereby establishing (5.1) in a direct way.

5.3 Second variation via partial EL equivalence

We now suppose that the map $\boldsymbol{y}(\boldsymbol{x})$ is Lipschitz continuous on Ω and of class C^2 everywhere, except on the smooth singular surface Σ, where the gradient $\boldsymbol{F}(\boldsymbol{x})=\nabla\boldsymbol{y}$ suffers a jump discontinuity. In this case the general second variation (3.19) reduces, according to Theorem 4.4, to the sum of $\delta^2 I_{\Omega\setminus\Sigma}(\boldsymbol{\psi},\boldsymbol{0})$ and a surface integral over Σ involving the cumulative variation $\boldsymbol{\psi}$.

THEOREM **5.2.** *Assume that the surface Σ of jump discontinuity of $\boldsymbol{F}(\boldsymbol{x})$ is orientable and has no boundary in Ω. Then*

$$\delta^2 I_\Omega(\boldsymbol{\phi},\boldsymbol{\theta}) = \delta^2 I_{\Omega\setminus\Sigma}(\boldsymbol{\psi},\boldsymbol{0}) - \mathfrak{S}, \tag{5.16}$$

where

$$\mathfrak{S} = \int_\Sigma \left[2([\![\boldsymbol{P}]\!],\nabla_\Sigma\{\!\!\{\boldsymbol{\psi}\}\!\!\})\xi + \left(\frac{\partial p^*}{\partial \boldsymbol{n}} - (\{\!\!\{L_{\boldsymbol{y}}\}\!\!\},[\![\boldsymbol{F}]\!]\boldsymbol{n})\right)\xi^2 + 2\xi([\![L_{\boldsymbol{y}}]\!],\{\!\!\{\boldsymbol{\psi}\}\!\!\})\right] dS,$$

and where we define $\partial p^*/\partial\boldsymbol{n}$ as the formal derivative of p^* in the direction $\boldsymbol{n}$:

$$\frac{\partial p^*}{\partial \boldsymbol{n}} \stackrel{\text{def}}{=} [\![\frac{\partial L}{\partial \boldsymbol{n}}]\!] - (\{\!\!\{\boldsymbol{P}\}\!\!\},[\![\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{n}}]\!]) - (\{\!\!\{\frac{\partial \boldsymbol{P}}{\partial \boldsymbol{n}}\}\!\!\},[\![\boldsymbol{F}]\!]). \tag{5.17}$$

Proof. First we choose a smooth unit normal field $\boldsymbol{n}(\boldsymbol{x})$, $\boldsymbol{x}\in\Sigma$. It is possible to partition Ω into two open sets Ω_+, Ω_- and Σ in such a way that the unit normal $\boldsymbol{n}(\boldsymbol{x})$ points from Ω_- into Ω_+ (see Section 5.1). It follows from Theorem 4.4, applied to Ω_+ and Ω_- that

$$\delta^2 I_\Omega(\boldsymbol{\phi},\boldsymbol{\theta}) = \delta^2 I_{\Omega\setminus\Sigma}(\boldsymbol{\psi},\boldsymbol{0}) - I_1 - I_2 - I_3,$$

where

$$I_1 = 2\int_\Sigma ([\![\boldsymbol{P}^T\nabla_\Sigma\boldsymbol{\psi}]\!],(\boldsymbol{\theta},\boldsymbol{n})\boldsymbol{I} - \boldsymbol{n}\otimes\boldsymbol{\theta})dS,$$

$$I_2 = \int_\Sigma ([\![\boldsymbol{P}^*]\!]^T\nabla_\Sigma\boldsymbol{\theta} + [\![\boldsymbol{P}^T\nabla_\Sigma(\boldsymbol{F}\boldsymbol{\theta})]\!],(\boldsymbol{\theta},\boldsymbol{n})\boldsymbol{I} - \boldsymbol{n}\otimes\boldsymbol{\theta})dS,$$

$$I_3 = \int_\Sigma \{[\![(L_{\boldsymbol{y}},2\boldsymbol{\psi}+\boldsymbol{F}\boldsymbol{\theta})]\!] + ([\![L_{\boldsymbol{x}}]\!],\boldsymbol{\theta})\}(\boldsymbol{\theta},\boldsymbol{n})dS.$$

Step 1. Let us simplify the first integral I_1. The jump of the product formula (5.5) and continuity of tractions (5.7) give

$$I_1 = 2\int_\Sigma ([\![\boldsymbol{P}]\!],\{\!\!\{\nabla_\Sigma\boldsymbol{\psi}\}\!\!\})\xi dS + I_1',$$

where

$$I_1' = 2\int_\Sigma \{\xi(\{\!\!\{\boldsymbol{P}\}\!\!\},\nabla_\Sigma[\![\boldsymbol{\psi}]\!]) - (\boldsymbol{P}\boldsymbol{n},(\nabla_\Sigma[\![\boldsymbol{\psi}]\!])\boldsymbol{\theta})\}dS.$$

Step 2. We decompose $\boldsymbol{\theta}(\boldsymbol{x})$ into its tangential and normal components

$$\boldsymbol{\theta} = \boldsymbol{\theta}_\tau + \xi\boldsymbol{n}, \tag{5.18}$$

and show that only the normal component ξ of $\boldsymbol{\theta}$ contributes to the second variation. In I_1' we eliminate $[\![\boldsymbol{\psi}]\!]$ by means of (5.9):

$$\nabla_\Sigma[\![\boldsymbol{\psi}]\!] = -[\![\boldsymbol{F}]\!]\boldsymbol{n}\otimes\nabla_\Sigma\xi - \xi\nabla_\Sigma([\![\boldsymbol{F}]\!]\boldsymbol{n}).$$

We claim that

$$\nabla_\Sigma([\![\boldsymbol{F}]\!]\boldsymbol{n}) = [\![\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{n}}]\!](\boldsymbol{I} - \boldsymbol{n} \otimes \boldsymbol{n}). \tag{5.19}$$

Indeed, using (4.18) we obtain

$$\nabla_\Sigma([\![\boldsymbol{F}]\!]\boldsymbol{n})_{i\beta} = [\![(F_{i\alpha,\beta} - F_{i\alpha,\gamma}n_\gamma n_\beta)n_\alpha]\!] + ([\![\boldsymbol{F}]\!]\nabla_\Sigma \boldsymbol{n})_{i\beta}.$$

The second term vanishes because the matrix $\nabla_\Sigma \boldsymbol{n}$ is symmetric and, by (5.6),

$$[\![\boldsymbol{F}]\!]\nabla_\Sigma \boldsymbol{n} = \boldsymbol{a} \otimes (\nabla_\Sigma \boldsymbol{n})^T \boldsymbol{n} = \boldsymbol{a} \otimes (\nabla_\Sigma \boldsymbol{n})\boldsymbol{n} = \boldsymbol{0}.$$

Recalling that $F_{i\alpha} = y_{i,\alpha}$ we conclude that

$$\nabla_\Sigma([\![\boldsymbol{F}]\!]\boldsymbol{n})_{i\beta} = [\![F_{i\beta,\alpha}n_\alpha - F_{i\alpha,\gamma}n_\gamma n_\beta n_\alpha]\!].$$

This formula is just (5.19) written out in components. We can now write

$$I_1' = 2\int_\Sigma \{(\boldsymbol{Pn}, [\![\boldsymbol{F}]\!]\boldsymbol{n})(\nabla_\Sigma \xi, \boldsymbol{\theta}_\tau) + \xi(\boldsymbol{Pn}, [\![\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{n}}]\!]\boldsymbol{\theta}_\tau) - \xi(\{\!\!\{\boldsymbol{P}\}\!\!\}\nabla_\Sigma \xi, [\![\boldsymbol{F}]\!]\boldsymbol{n})$$
$$- \xi^2(\{\!\!\{\boldsymbol{P}\}\!\!\}, [\![\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{n}}]\!]) + \xi^2(\boldsymbol{Pn}, [\![\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{n}}]\!]\boldsymbol{n})\}dS.$$

Step 3. Consider now the integral I_2. In order to simplify it we need to use a well-known relation

$$[\![\boldsymbol{P}^*]\!]\boldsymbol{n} = p^*\boldsymbol{n}, \tag{5.20}$$

which is a consequence of the application of the jump of the product formula (5.5) and kinematic compatibility relation (5.6) to the definition (3.7) of $\boldsymbol{P}^*$. Using (5.5), (5.7), (5.8) and (5.20) we can write $I_2 = I_{21} + I_{22}$, where

$$I_{21} = \int_\Sigma (\{\!\!\{\boldsymbol{P}\}\!\!\}(\xi \boldsymbol{I} - \boldsymbol{n} \otimes \boldsymbol{\theta}), \nabla_\Sigma([\![\boldsymbol{F}]\!]\boldsymbol{\theta}))dS,$$

$$I_{22} = \int_\Sigma \big(\xi([\![\boldsymbol{P}_*]\!], \nabla_\Sigma \boldsymbol{\theta}) + \xi([\![\boldsymbol{P}]\!], \nabla_\Sigma(\{\!\!\{\boldsymbol{F}\}\!\!\}\boldsymbol{\theta}))\big)dS.$$

Simplifying the integral I_{21} using (5.6) and (5.19) and expanding, we obtain

$$I_{21} = \int_\Sigma \Big(\xi^2(\{\!\!\{\boldsymbol{P}\}\!\!\}, [\![\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{n}}]\!]) - \xi^2(\boldsymbol{Pn}, [\![\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{n}}]\!]\boldsymbol{n})$$
$$- \xi(\boldsymbol{Pn}, [\![\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{n}}]\!]\boldsymbol{\theta}_\tau) - ([\![\boldsymbol{F}]\!]\boldsymbol{n}, \boldsymbol{Pn})(\nabla_\Sigma \xi, \boldsymbol{\theta}_\tau) + \xi([\![\boldsymbol{F}]\!]\boldsymbol{n}, \{\!\!\{\boldsymbol{P}\}\!\!\}\nabla_\Sigma \xi)\Big)dS.$$

Next, we integrate by parts in I_{22}. We use the following integration by parts formula

$$\int_\Sigma (\boldsymbol{f}, \nabla_\Sigma \phi)dS(\boldsymbol{x}) = \int_\Sigma \{\phi(\boldsymbol{f}, \boldsymbol{n})\nabla_\Sigma \cdot \boldsymbol{n} - \phi \nabla_\Sigma \cdot \boldsymbol{f}\}dS, \tag{5.21}$$

which holds provided, either $\boldsymbol{f}$ or ϕ vanishes at every point on the boundary of Σ (which is on $\partial\Omega$ by assumption). We obtain

$$I_{22} = \int_\Sigma \Big(\xi^2[\![\frac{\partial L}{\partial \boldsymbol{n}}]\!] - \xi^2(\boldsymbol{P}\boldsymbol{n},[\![\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{n}}]\!]\boldsymbol{n}) - \xi^2([\![\boldsymbol{F}]\!]\boldsymbol{n},\{\!\!\{\frac{\partial \boldsymbol{P}}{\partial \boldsymbol{n}}\}\!\!\}\boldsymbol{n}) - \xi(\boldsymbol{P}\boldsymbol{n},[\![\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{n}}]\!]\boldsymbol{\theta}_\tau) -$$
$$[\![L]\!](\nabla_\Sigma\xi,\boldsymbol{\theta}_\tau) + \xi([\![\boldsymbol{F}]\!]\boldsymbol{n},\{\!\!\{\boldsymbol{P}\}\!\!\}\nabla_\Sigma\xi) - \xi([\![L_{\boldsymbol{x}}]\!],\boldsymbol{\theta}) - \xi([\![L_{\boldsymbol{y}}]\!],\{\!\!\{\boldsymbol{F}\}\!\!\}\boldsymbol{\theta})\Big)dS,$$

where we have also used (5.7), (5.20), and the following equations

$$\nabla_\Sigma\cdot\boldsymbol{P} = \nabla\cdot\boldsymbol{P} - \frac{\partial \boldsymbol{P}}{\partial \boldsymbol{n}}\boldsymbol{n} = L_{\boldsymbol{y}} - \frac{\partial \boldsymbol{P}}{\partial \boldsymbol{n}}\boldsymbol{n}, \tag{5.22}$$

$$\nabla_\Sigma\cdot\boldsymbol{P}_* = \nabla\cdot\boldsymbol{P}_* - \frac{\partial \boldsymbol{P}_*}{\partial \boldsymbol{n}}\boldsymbol{n} = L_{\boldsymbol{x}} - \frac{\partial \boldsymbol{P}_*}{\partial \boldsymbol{n}}\boldsymbol{n} = L_{\boldsymbol{x}} - \frac{\partial L}{\partial \boldsymbol{n}}\boldsymbol{n} + \frac{\partial \boldsymbol{F}^T}{\partial \boldsymbol{n}}\boldsymbol{P}\boldsymbol{n} + \boldsymbol{F}^T\frac{\partial \boldsymbol{P}}{\partial \boldsymbol{n}}\boldsymbol{n}.$$

Adding the integrals I_{21} and I_{22}, taking into account that $[\![L]\!] = ([\![\boldsymbol{F}]\!]\boldsymbol{n},\boldsymbol{P}\boldsymbol{n})$, we obtain

$$I_2 = \int_\Sigma \Big(\xi^2[\![\frac{\partial L}{\partial \boldsymbol{n}}]\!] + \xi^2(\{\!\!\{\boldsymbol{P}\}\!\!\},[\![\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{n}}]\!]) - 2\xi^2(\boldsymbol{P}\boldsymbol{n},[\![\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{n}}]\!]\boldsymbol{n}) - \xi^2([\![\boldsymbol{F}]\!]\boldsymbol{n},\{\!\!\{\frac{\partial \boldsymbol{P}}{\partial \boldsymbol{n}}\}\!\!\}\boldsymbol{n}) - 2\xi(\boldsymbol{P}\boldsymbol{n},[\![\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{n}}]\!]\boldsymbol{\theta}_\tau)$$
$$- 2([\![\boldsymbol{F}]\!]\boldsymbol{n},\boldsymbol{P}\boldsymbol{n})(\nabla_\Sigma\xi,\boldsymbol{\theta}_\tau) + 2\xi([\![\boldsymbol{F}]\!]\boldsymbol{n},\{\!\!\{\boldsymbol{P}\}\!\!\}\nabla_\Sigma\xi) - \xi([\![L_{\boldsymbol{x}}]\!],\boldsymbol{\theta}) - \xi([\![L_{\boldsymbol{y}}]\!],\{\!\!\{\boldsymbol{F}\}\!\!\}\boldsymbol{\theta})\Big)dS.$$

Adding I_1' and I_2 we get, by virtue of

$$([\![\boldsymbol{F}]\!]\boldsymbol{n},\{\!\!\{\frac{\partial \boldsymbol{P}}{\partial \boldsymbol{n}}\}\!\!\}\boldsymbol{n}) = ([\![\boldsymbol{F}]\!],\{\!\!\{\frac{\partial \boldsymbol{P}}{\partial \boldsymbol{n}}\}\!\!\}),$$

that, due to (5.6),

$$I_1' + I_2 = \int_\Sigma \left\{\xi^2\frac{\partial p^*}{\partial \boldsymbol{n}} - \xi([\![L_{\boldsymbol{x}}]\!],\boldsymbol{\theta}) - \xi([\![L_{\boldsymbol{y}}]\!],\{\!\!\{\boldsymbol{F}\}\!\!\}\boldsymbol{\theta})\right\}dS,$$

where we have used the definition (5.17) of $\partial p^*/\partial\boldsymbol{n}$.

Step 4. Using the product rule formula (5.5) we obtain

$$I_3 = \int_\Sigma \{\xi([\![L_{\boldsymbol{x}}]\!],\boldsymbol{\theta}) + 2\xi([\![L_{\boldsymbol{y}}]\!],\{\!\!\{\boldsymbol{\psi}\}\!\!\}) + \xi([\![L_{\boldsymbol{y}}]\!],\{\!\!\{\boldsymbol{F}\}\!\!\}\boldsymbol{\theta}) + 2\xi(\{\!\!\{L_{\boldsymbol{y}}\}\!\!\},[\![\boldsymbol{\psi}]\!]) + \xi(\{\!\!\{L_{\boldsymbol{y}}\}\!\!\},[\![\boldsymbol{F}]\!]\boldsymbol{\theta})\}dS.$$

Recalling the formulas (5.6) and (5.9), we finally obtain

$$I_1' + I_2 + I_3 = \int_\Sigma \left\{\xi^2\left(\frac{\partial p^*}{\partial \boldsymbol{n}} - (\{\!\!\{L_{\boldsymbol{y}}\}\!\!\},[\![\boldsymbol{F}]\!]\boldsymbol{n})\right) + 2\xi([\![L_{\boldsymbol{y}}]\!],\{\!\!\{\boldsymbol{\psi}\}\!\!\})\right\}dS.$$

Theorem 5.2 is now proved. □

It appears, as though the contribution of the surface Σ to the second variation depends on the extension of $\boldsymbol{F}(\boldsymbol{x})$ into $\Omega\setminus\Sigma$ via the term $\xi^2\partial p^*/\partial\boldsymbol{n}$. This is not so because $\partial p^*/\partial\boldsymbol{n}$ depends only on the traces $\boldsymbol{F}_\pm$ of $\boldsymbol{F}(\boldsymbol{x})$ on Σ and their tangential derivatives $\nabla_\Sigma\boldsymbol{F}_\pm$:

$$\frac{\partial p^*}{\partial \boldsymbol{n}} = ([\![\boldsymbol{P}]\!],\nabla_\Sigma(\{\!\!\{\boldsymbol{F}\}\!\!\}\boldsymbol{n}) - \{\!\!\{\boldsymbol{F}\}\!\!\}\nabla_\Sigma\boldsymbol{n}) + (\nabla_\Sigma\cdot\{\!\!\{\boldsymbol{P}\}\!\!\},[\![\boldsymbol{F}]\!]\boldsymbol{n}) + ([\![L_{\boldsymbol{x}}]\!],\boldsymbol{n}) + ([\![L_{\boldsymbol{y}}]\!],\{\!\!\{\boldsymbol{F}\}\!\!\}\boldsymbol{n}).$$

In particular, if $L(\boldsymbol{x},\boldsymbol{y},\boldsymbol{F}) = W(\boldsymbol{F})$, the surface Σ is planar and $\boldsymbol{F}(\boldsymbol{x})$ is constant along Σ, then $\dfrac{\partial p^*}{\partial \boldsymbol{n}} = 0$.

5.4 Second variation via full EL equivalence

We now derive the formula (5.16) directly by using the explicit structure (5.14) of the EL equivalent strong outer variation $\boldsymbol{\phi}_\epsilon$ introduced in (2.8).

Here we assume that the first variation $\delta I_\Omega(\boldsymbol{\phi}, \boldsymbol{\theta})$ vanishes. In order to derive the formula for the second variation we simply use the technique of Section 5.2, while carrying the expansion of the energy increment to the second order in ϵ. We have

$$I(\boldsymbol{y}_\epsilon) - I(\boldsymbol{y}) = \int_{V_\Sigma(\epsilon)} L^\star d\boldsymbol{x} + \int_{\Omega\setminus V_\Sigma(\epsilon)} L^\star d\boldsymbol{x}, \tag{5.23}$$

On $\Omega \setminus V_\Sigma(\epsilon)$ the variation $\boldsymbol{\phi}_\epsilon$ given by (5.15) is equivalent to $\epsilon\boldsymbol{\psi}$, and therefore,

$$\lim_{\epsilon\to 0} \frac{1}{\epsilon^2} \int_{\Omega\setminus V_\Sigma(\epsilon)} L^\star d\boldsymbol{x} = \frac{1}{2}\delta^2 I_{\Omega\setminus\Sigma}(\boldsymbol{\psi}, \boldsymbol{0}). \tag{5.24}$$

To expand the second term in (5.23) we need to expand $L^\star$ to the first order in ϵ, since the set $V_\Sigma(\epsilon)$ has $O(\epsilon)$ measure. This is done using the formulas (5.11), (5.14) and (5.15). If $\boldsymbol{x} \in V_\Sigma^\pm(\epsilon)$, then

$$L^\star = \mp p^* \mp z\left[[\![\frac{\partial L}{\partial \boldsymbol{n}}]\!] - (\frac{\partial \boldsymbol{P}_\pm}{\partial \boldsymbol{n}}, [\![\boldsymbol{F}]\!]) - (\boldsymbol{P}_\pm, [\![\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{n}}]\!]) - (L_{\boldsymbol{y}}^\pm, [\![\boldsymbol{F}]\!]\boldsymbol{n}) \right] \\ \mp \epsilon[([\![\boldsymbol{P}]\!], \nabla\boldsymbol{\psi}_\mp) + ([\![L_{\boldsymbol{y}}]\!], \boldsymbol{\psi}_\mp)] + o(\epsilon).$$

The Maxwell relation $p^* = 0$ then implies that $L^\star = O(\epsilon)$. Therefore,

$$\int_{V_\Sigma^\pm(\epsilon)} L^\star d\boldsymbol{x} = -\frac{\epsilon^2}{2}\int_{\Sigma_\pm} \Lambda^\pm dS + o(\epsilon^2),$$

where

$$\Lambda^\pm = \xi^2\left[[\![\frac{\partial L}{\partial \boldsymbol{n}}]\!] - (\frac{\partial \boldsymbol{P}_\pm}{\partial \boldsymbol{n}}, [\![\boldsymbol{F}]\!]) - (\boldsymbol{P}_\pm, [\![\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{n}}]\!]) - (L_{\boldsymbol{y}}^\pm, [\![\boldsymbol{F}]\!]\boldsymbol{n}) \right] \\ + 2\xi[([\![\boldsymbol{P}]\!], \nabla_\Sigma\boldsymbol{\psi}_\mp) + ([\![L_{\boldsymbol{y}}]\!], \boldsymbol{\psi}_\mp)].$$

It remains to observe that

$$\int_{\Sigma_\pm} [\![\Lambda]\!](\boldsymbol{u}) dS(\boldsymbol{u}) = 0. \tag{5.25}$$

Indeed,

$$-[\![\Lambda]\!] = \xi^2\left[([\![\frac{\partial \boldsymbol{P}}{\partial \boldsymbol{n}}]\!], [\![\boldsymbol{F}]\!]) + ([\![\boldsymbol{P}]\!], [\![\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{n}}]\!]) + ([\![L_{\boldsymbol{y}}]\!], [\![\boldsymbol{F}]\!]\boldsymbol{n}) \right] + 2\xi[([\![\boldsymbol{P}]\!], \nabla_\Sigma[\![\boldsymbol{\psi}]\!]) + ([\![L_{\boldsymbol{y}}]\!], [\![\boldsymbol{\psi}]\!])].$$

We can now use (5.9) and the relations

$$([\![\frac{\partial \boldsymbol{P}}{\partial \boldsymbol{n}}]\!], [\![\boldsymbol{F}]\!]) = ([\![L_{\boldsymbol{y}}]\!], [\![\boldsymbol{F}]\!]\boldsymbol{n}) - (\nabla_\Sigma \cdot [\![\boldsymbol{P}]\!], [\![\boldsymbol{F}]\!]\boldsymbol{n}),$$

which follows from (5.22), and

$$([\![\boldsymbol{P}]\!],[\![\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{n}}]\!])=([\![\boldsymbol{P}]\!],\nabla_{\Sigma}([\![\boldsymbol{F}]\!]\boldsymbol{n})).$$

which follows from (5.19) and (5.7) to obtain

$$[\![\Lambda]\!]=\nabla_{\Sigma}\cdot(\xi^{2}[\![\boldsymbol{P}]\!]^{T}[\![\boldsymbol{F}]\!]\boldsymbol{n}).$$

The desired relation (5.25) follows from the fact that due to (5.7) the vector field $\xi^2[\![\boldsymbol{P}]\!]^T[\![\boldsymbol{F}]\!]\boldsymbol{n}$ is tangent to Σ and ξ vanishes on the boundaries of $\Sigma_{\pm}$ (since, these boundaries are either points where ξ changes sign or points on $\partial\Omega$, where ξ vanishes). Moreover, regardless of the boundary values of ξ, the expression $[\![\boldsymbol{P}]\!]^T[\![\boldsymbol{F}]\!]\boldsymbol{n}$ must necessarily vanish for stable jump discontinuities, as we have recently shown in [26]. In any case we obtain, using (5.17), that

$$\lim_{\epsilon\to 0}\frac{1}{\epsilon^{2}}\int_{V_{\Sigma}(\epsilon)}L^{\star}d\boldsymbol{x}=-\int_{\Sigma}\Bigg[([\![\boldsymbol{P}]\!],\nabla_{\Sigma}\{\!\!\{\boldsymbol{\psi}\}\!\!\})\xi + \frac{1}{2}\left(\frac{\partial p^{*}}{\partial \boldsymbol{n}}-(\{\!\!\{L_{\boldsymbol{y}}\}\!\!\},[\![\boldsymbol{F}]\!]\boldsymbol{n})\right)\xi^{2}+\xi([\![L_{\boldsymbol{y}}]\!],\{\!\!\{\boldsymbol{\psi}\}\!\!\})\Bigg]dS,$$

Combining this relation with (5.24) we obtain the result (5.16).

The link between the formula (5.16) and the calculations of Grinfeld [29] who used the Weierstrass-Erdmann technique is discussed in the Appendix A.

6 Global necessary conditions

6.1 General conditions

If $\boldsymbol{y}(\boldsymbol{x})$ is a strong local minimizer, then the first variation $\delta I(\boldsymbol{\phi},\boldsymbol{\theta})$ must vanish, while the second variation $\delta^2 I_\Omega(\boldsymbol{\phi},\boldsymbol{\theta})$ must be non-negative.

The condition of vanishing of the first variation leads to two types of equations

$$\delta I_{\Omega}(\boldsymbol{\phi},\boldsymbol{0})=\int_{\Omega}\{(L_{\boldsymbol{y}},\boldsymbol{\phi})+(\boldsymbol{P},\nabla\boldsymbol{\phi})\}d\boldsymbol{x}=0, \tag{6.1}$$

for all $\boldsymbol{\phi}\in$ Var, and

$$\delta I_{\Omega}(\boldsymbol{0},\boldsymbol{\theta})=\int_{\Omega}\{(L_{\boldsymbol{x}},\boldsymbol{\theta})+(\boldsymbol{P}^{*},\nabla\boldsymbol{\theta})\}d\boldsymbol{x}=0, \tag{6.2}$$

for all $\boldsymbol{\theta}\in C^2(\overline{\Omega};\mathbb{R}^d)\cap C_0(\Omega;\mathbb{R}^d)$. For general Lipschitz extremals these two equations should be regarded as independent. By contrast, in the case of C^2 extremals, (6.2) becomes a corollary of (6.1).

In the case of interest, when singularities are present, the Eshelby equation (6.2) reduces to conditions localized at the singular set. For example, when $\boldsymbol{y}(\boldsymbol{x})$ is of class C^2, except on a smooth surface of jump discontinuity for $\boldsymbol{F}(\boldsymbol{x})$, equations (6.1) and (6.2) produce additional jump conditions: the continuity of tractions $[\![\boldsymbol{P}]\!]\boldsymbol{n} = \boldsymbol{0}$ and the Maxwell relation

$$[\![L]\!] - (\{\!\!\{\boldsymbol{P}\}\!\!\}, [\![\boldsymbol{F}]\!]) = 0. \tag{6.3}$$

If the singular set Σ has co-dimension larger than 1, then there exists a family D_ϵ of smooth subdomains of Ω such that $|\Omega \setminus D_\epsilon| \to 0$, as $\epsilon \to 0$, $\Sigma \subset \Omega \setminus D_\epsilon$ and the surface area of ∂D_ϵ goes to zero. Then, the boundedness of $\boldsymbol{F}(\boldsymbol{x})$ implies

$$\delta I_\Omega(\boldsymbol{\phi}, \boldsymbol{\theta}) = \lim_{\epsilon \to 0} \delta I_{D_\epsilon}(\boldsymbol{\phi}, \boldsymbol{\theta}).$$

Applying Theorem 4.3 with $D = D_\epsilon$ we obtain

$$\delta I_\Omega(\boldsymbol{\phi}, \boldsymbol{\theta}) = \lim_{\epsilon \to 0} \left\{ \delta I_{D_\epsilon}(\boldsymbol{\psi}, \boldsymbol{0}) + \int_{\partial D_\epsilon} L(\boldsymbol{\theta}, \boldsymbol{n}) dS \right\}.$$

Since the surface area of ∂D_ϵ goes to zero, we obtain $\delta I_\Omega(\boldsymbol{\phi}, \boldsymbol{\theta}) = \delta I_{\Omega \setminus \Sigma}(\boldsymbol{\psi}, \boldsymbol{0})$. In other words, the weak form of the Eshelby equation (6.2) is a consequence of the weak form of the Euler-Lagrange equation (6.1), and the variational functional "does not see" singularities of co-dimension more than 1 at the level of first variation. By contrast, the method above can provide non-trivial information about singularities with *unbounded* $\boldsymbol{F}(\boldsymbol{x})$ (e.g. [8]).

We now turn to the condition of non-negativity of second variation. In the general case we can use (3.19) to obtain

$$\int_\Omega \{2J_2(\nabla \boldsymbol{\theta})L + 2((L_{\boldsymbol{x}}, \boldsymbol{\theta}) + (L_{\boldsymbol{y}}, \boldsymbol{\phi}))\nabla \cdot \boldsymbol{\theta} + (L_{\boldsymbol{xx}}\boldsymbol{\theta}, \boldsymbol{\theta}) + (L_{\boldsymbol{yy}}\boldsymbol{\phi}, \boldsymbol{\phi}) + 2(L_{\boldsymbol{xy}}\boldsymbol{\phi}, \boldsymbol{\theta}) \\ + 2(\boldsymbol{P}\boldsymbol{\Theta}(\nabla \boldsymbol{\theta}), \boldsymbol{H}) + (L_{\boldsymbol{FF}}\boldsymbol{H}, \boldsymbol{H}) + 2(L_{\boldsymbol{Fx}}\boldsymbol{\theta} + L_{\boldsymbol{Fy}}\boldsymbol{\phi}, \boldsymbol{H})\} d\boldsymbol{x} \geq 0. \tag{6.4}$$

This inequality has to hold for every choice of $\boldsymbol{\phi} \in \mathrm{Var}$ and $\boldsymbol{\theta} \in C^1(\overline{\Omega}; \mathbb{R}^d) \cap C_0(\Omega; \mathbb{R}^d)$. If $\boldsymbol{y} \in C^2(\overline{\Omega}; \mathbb{R}^m)$ then the non-negativity of (3.19) is equivalent to the non-negativity of the classical second variation:

$$\delta^2 I_\Omega(\boldsymbol{\phi}, \boldsymbol{0}) = \int_\Omega \{(L_{\boldsymbol{yy}}\boldsymbol{\phi}, \boldsymbol{\phi}) + (L_{\boldsymbol{FF}}\nabla \boldsymbol{\phi}, \nabla \boldsymbol{\phi}) + 2(L_{\boldsymbol{Fy}}\boldsymbol{\phi}, \nabla \boldsymbol{\phi})\} d\boldsymbol{x} \geq 0. \tag{6.5}$$

In the case of a smooth surface of jump discontinuity, condition (6.4) reduces to

$$\int_\Omega \{(L_{\boldsymbol{yy}}\boldsymbol{\psi}, \boldsymbol{\psi}) + (L_{\boldsymbol{FF}}\widetilde{\nabla}\boldsymbol{\psi}, \widetilde{\nabla}\boldsymbol{\psi}) + 2(L_{\boldsymbol{Fy}}\boldsymbol{\psi}, \widetilde{\nabla}\boldsymbol{\psi})\} d\boldsymbol{x} - \int_\Sigma \{2([\![\boldsymbol{P}]\!], \nabla_\Sigma \{\!\!\{\boldsymbol{\psi}\}\!\!\})\xi + \\ \left(\frac{\partial p^*}{\partial \boldsymbol{n}} - (\{\!\!\{L_{\boldsymbol{y}}\}\!\!\}, [\![\boldsymbol{F}]\!]\boldsymbol{n}) \right) \xi^2 + 2\xi([\![L_{\boldsymbol{y}}]\!], \{\!\!\{\boldsymbol{\psi}\}\!\!\})\} dS \geq 0, \tag{6.6}$$

where $\widetilde{\nabla}\boldsymbol{\psi}$ is the regular part of the gradients of the discontinuous function $\boldsymbol{\psi}$. The surface term containing $[\![\boldsymbol{P}]\!]$, represents the prestress of the interface and can have a destabilizing effect, capable of making the second variation negative, even when the tangential elasticity tensor $L_{\boldsymbol{FF}}(\boldsymbol{x})$ is uniformly positive definite (see the example in Section 6.2).

If $\boldsymbol{F}(\boldsymbol{x})$ is singular on a set of higher co-dimension, we proceed as in the case of the first variation, to obtain

$$\delta^2 I_\Omega(\boldsymbol{\phi},\boldsymbol{\theta}) = \lim_{\epsilon\to 0}\delta^2 I_{D_\epsilon}(\boldsymbol{\phi},\boldsymbol{\theta}).$$

We then apply Theorem 4.4 and conclude that EL equivalence principle

$$\delta^2 I_\Omega(\boldsymbol{\phi},\boldsymbol{\theta}) = \delta^2 I_{\Omega\setminus\Sigma}(\boldsymbol{\psi},\boldsymbol{0}) \tag{6.7}$$

holds, provided $|\nabla\boldsymbol{F}(\boldsymbol{x})|\epsilon^{k-1}\to 0$, when the distance between $\boldsymbol{x}$ and Σ is ϵ, and k is the co-dimension of Σ. If $|\nabla\boldsymbol{F}|$ grows faster as we approach the singularity then we may not conclude that (6.7) holds, because

$$\lim_{\epsilon\to 0}\int_{\partial D_\epsilon}(\nabla_{\partial D_\epsilon}(\boldsymbol{F}\boldsymbol{\theta}),\boldsymbol{P}((\boldsymbol{\theta},\boldsymbol{n})\boldsymbol{I}-\boldsymbol{n}\otimes\boldsymbol{\theta}))dS$$

might be non-zero.

This analysis shows that certain singularities of higher co-dimension may be "invisible" by the functional $I(\boldsymbol{y})$. This may explain the surprising counterexamples to regularity in vectorial variational problems [44, 54] in high dimensions.

6.2 Example

In this example we deal with an equilibrium configuration whose instability can at present be only detected by examining the global inner-outer second variation (5.16).

Consider the vectorial 2D problem with the double-well energy density $L(\boldsymbol{F})$ in the form $L(\boldsymbol{F}) = W(\boldsymbol{\varepsilon})$, where $\boldsymbol{\varepsilon} = (\boldsymbol{F}+\boldsymbol{F}^T)/2$ and $\boldsymbol{F}$ is a 2×2 matrix. This energy density comes from the problem of finding energy-minimizing composite materials [34]. Assume that

$$W(\boldsymbol{\varepsilon}) = \min\{f_+(\boldsymbol{\varepsilon}), f_-(\boldsymbol{\varepsilon})\},\qquad f_\pm(\boldsymbol{\varepsilon}) = \frac{1}{2}(\mathsf{C}_\pm\boldsymbol{\varepsilon},\boldsymbol{\varepsilon}) + w_\pm, \tag{6.8}$$

where $\boldsymbol{\varepsilon}\in \mathrm{Sym}(\mathbb{R}^2)$ and the two isotropic phases have different elastic moduli

$$\mathsf{C}_\pm\boldsymbol{\varepsilon} = \kappa_\pm(\mathrm{Tr}\,\boldsymbol{\varepsilon})\boldsymbol{I} + 2\mu_\pm\left(\boldsymbol{\varepsilon} - \frac{1}{2}(\mathrm{Tr}\,\boldsymbol{\varepsilon})\boldsymbol{I}\right)$$

with $\kappa_+ > \kappa_- > 0$, $\mu_+ > \mu_- > 0$.

Remark 6.1. *If the transformation strains $\boldsymbol{\varepsilon}^\circ_\pm$ are present, they can be eliminated by a simple affine transformation, provided $[\![\mathsf{C}]\!]$ is invertible [12, 43, 21]. It is enough to observe that if*

$$\widehat{W}(\boldsymbol{\varepsilon}) = \min\{\frac{1}{2}(\mathsf{C}_+(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^\circ_+),\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^\circ_+) + \widehat{w}_+, \frac{1}{2}(\mathsf{C}_-(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^\circ_-),\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^\circ_-) + \widehat{w}_-\} \tag{6.9}$$

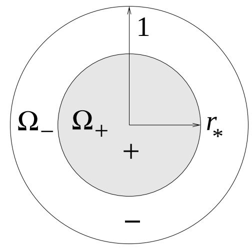

Figure 3: The heterogeneous disc

then

$$\widehat{W}(\boldsymbol{\varepsilon}) = W(\boldsymbol{\varepsilon} - \overline{\boldsymbol{\varepsilon}}) + (\boldsymbol{\sigma}^\circ, \boldsymbol{\varepsilon}) - \frac{1}{2}(\boldsymbol{\sigma}^\circ, \overline{\boldsymbol{\varepsilon}}),$$

where

$$\overline{\boldsymbol{\varepsilon}} = [\![\mathsf{C}]\!]^{-1}[\![\mathsf{C}\boldsymbol{\varepsilon}^\circ]\!], \qquad \boldsymbol{\sigma}^\circ = \{\!\!\{\mathsf{C}\}\!\!\}\overline{\boldsymbol{\varepsilon}} - \{\!\!\{\mathsf{C}\boldsymbol{\varepsilon}^\circ\}\!\!\} = \mathsf{C}_\pm(\overline{\boldsymbol{\varepsilon}} - \boldsymbol{\varepsilon}^\circ_\pm), \qquad w_\pm = \widehat{w}_\pm - \frac{1}{2}(\boldsymbol{\sigma}^\circ, \boldsymbol{\varepsilon}^\circ_\pm).$$

Therefore the double-well energy (6.9) is equivalent to the energy (6.8).

Assume that Ω is the unit disk, which is loaded by uniform pressure $\boldsymbol{\sigma n} = p_0\boldsymbol{n}$ (see Figure 3). Consider the radially symmetric equilibrium configuration

$$\boldsymbol{y}(\boldsymbol{x}) = \begin{cases} \alpha_+\boldsymbol{x}, & \text{if } |\boldsymbol{x}| \le r_*, \\ \left(\alpha_- + \dfrac{\beta_-}{r^2}\right)\boldsymbol{x}, & \text{if } r_* \le |\boldsymbol{x}| \le 1 \end{cases}$$

with the two phases located at $0 < r < r_*$ and $r_* < r < 1$. It will be convenient to denote

$$\gamma(r) = \frac{\beta_-}{r^2}, \qquad \gamma_* = \frac{\beta_-}{r_*^2}.$$

The continuity of displacements and tractions on the gradient discontinuity $r = r_*$ are equivalent to

$$[\![\alpha]\!] = \gamma_*, \qquad [\![\kappa\alpha]\!] = -\mu_-\gamma_*, \tag{6.10}$$

respectively. Solving for $\alpha_\pm$ we obtain

$$\alpha_\pm = -\frac{\gamma_*}{[\![\kappa]\!]}(\kappa_\mp + \mu_-).$$

The Maxwell condition can be written as

$$p^* = \frac{1}{2}([\![\boldsymbol{\sigma}]\!], \{\!\!\{\boldsymbol{\varepsilon}\}\!\!\}) - \frac{1}{2}(\{\!\!\{\boldsymbol{\sigma}\}\!\!\}, [\![\boldsymbol{\varepsilon}]\!]) + [\![w]\!] = 0. \tag{6.11}$$

Eliminating $\alpha_\pm$ from (6.10) and substituting into (6.11) we obtain the equation for γ_*

$$2(\kappa_- + \mu_-)(\kappa_+ + \mu_-)\gamma_*^2 + [\![w]\!][\![\kappa]\!] = 0. \tag{6.12}$$

Finally, the pressure boundary conditions on $|\boldsymbol{x}| = 1$ result, after a simple computation, using (6.10), in

$$p_0 = -2\gamma_* \left(\kappa_- \frac{\kappa_+ + \mu_-}{[\![\kappa]\!]} + \mu_- r_*^2\right). \tag{6.13}$$

We see that among the two solutions γ_* of (6.12) we need to choose the one with the sign opposite to p_0. If we substitute that value of γ_* from (6.12) into (6.13) we will obtain the equation for r_*. The inequality $0 < r_* < 1$ implies the restrictions on the values of p_0 for which the heterogeneous configuration shown in Figure 3 is possible:

$$2|\gamma_*|\kappa_- \frac{\kappa_+ + \mu_-}{[\![\kappa]\!]} \le |p_0| \le 2|\gamma_*|\kappa_+ \frac{\kappa_- + \mu_-}{[\![\kappa]\!]}.$$

Once r_* are γ_* are determined the parameters $\alpha_\pm$ and $\beta_- = \gamma_* r_*^2$ are also determined.

We will now examine the global stability condition (5.16) on the fields

$$\boldsymbol{\psi}(\boldsymbol{x}) = \begin{cases} A_+ \boldsymbol{x}, & \text{if } |\boldsymbol{x}| \le r_*, \\ \left(A_- + \dfrac{B_-}{r^2}\right)\boldsymbol{x}, & \text{if } r_* \le |\boldsymbol{x}| \le 1, \end{cases} \tag{6.14}$$

By using an auxiliary condition $(\mathsf{C}_- \nabla \boldsymbol{\psi})\boldsymbol{n} = \boldsymbol{0}$ on $|\boldsymbol{x}| = 1$ we obtain

$$\boldsymbol{\psi}(\boldsymbol{x}) = \begin{cases} A_+ \boldsymbol{x}, & \text{if } |\boldsymbol{x}| \le r_*, \\ A_- \left(1 + \dfrac{\kappa_-}{\mu_- r^2}\right)\boldsymbol{x}, & \text{if } r_* \le |\boldsymbol{x}| \le 1. \end{cases}$$

We can now compute

$$E_+ = \int_{\Omega_+} (\mathsf{C}_+ \nabla \boldsymbol{\psi}, \nabla \boldsymbol{\psi}) d\boldsymbol{x} = 4\pi r_*^2 \kappa_+ A_+^2.$$

$$E_- = \int_{\Omega_-} (\mathsf{C}_- \nabla \boldsymbol{\psi}, \nabla \boldsymbol{\psi}) d\boldsymbol{x} = 4\pi (1 - r_*^2) \kappa_- A_-^2 \left(1 + \frac{\kappa_-}{\mu_- r_*^2}\right).$$

On $|\boldsymbol{x}| = r_*$ we obtain

$$[\![\boldsymbol{\psi}]\!] = \left(A_+ - A_- \left(1 + \frac{\kappa_-}{\mu_- r_*^2}\right)\right)\boldsymbol{x},$$

while $[\![\boldsymbol{\varepsilon}]\!]\boldsymbol{n} = -(2\gamma_*/r_*)\boldsymbol{x}$. Therefore, according to (5.9),

$$\xi = \frac{r_*}{2\gamma_*}\left(A_+ - A_- \left(1 + \frac{\kappa_-}{\mu_- r_*^2}\right)\right).$$

By using

$$[\![\boldsymbol{\sigma}]\!] = -4\mu_- \gamma_* (\boldsymbol{I} - \widehat{\boldsymbol{x}} \otimes \widehat{\boldsymbol{x}}). \tag{6.15}$$

we obtain

$$S_1 = 2\int_{|\boldsymbol{x}|=r_*} ([\![\boldsymbol{\sigma}]\!], \{\!\!\{ \widetilde{\nabla}\boldsymbol{\psi} \}\!\!\})\xi dS(\boldsymbol{x}) = -4\pi r_*^2 \mu_- \left(A_+^2 - A_-^2 \left(1 + \frac{\kappa_-}{\mu_- r_*^2} \right)^2 \right).$$

We compute $\dfrac{\partial p^*}{\partial \boldsymbol{n}} = 0$, and therefore, $S_2 = 0$. Thus, we obtain

$$\frac{\delta^2 I_\Omega(\boldsymbol{\psi}, \boldsymbol{0})}{4\pi} = r_*^2(\kappa_+ + \mu_-)A_+^2 - r_*^2(\kappa_- + \mu_-)A_-^2 \left(1 + \frac{\kappa_-}{\mu_- r_*^2} \right).$$

The quadratic form $\delta^2 I_\Omega$ is always indefinite. Therefore, the radially symmetric heterogeneous configurations in the unit ball are always unstable. Since the instability is with respect to radial variations, it can also be detected using the method of Lifshitz and Gulida [39, 38], where a radial equilibrium boundary value problem is solved and the second derivative of the energy at the equilibrium r_*, given by the Maxwell relation, is computed.

In a companion paper [23] we show that the extremal tested in this example satisfies both the quasiconvexity and the classical second variation conditions. Local stability condition, derived in the next section, is therefore, also satisfied.

7 Local necessary conditions

7.1 General conditions

We recall that in classical calculus of variations the Legendre-Hadamard condition is the localization of classical second variation condition $\delta^2 I_\Omega(\boldsymbol{\phi}, \boldsymbol{0}) \ge 0$. If we take a sequence of test functions

$$\boldsymbol{\phi}_\epsilon(\boldsymbol{x}) = \epsilon \boldsymbol{\phi}_0((\boldsymbol{x} - \boldsymbol{x}_0)/\epsilon), \tag{7.1}$$

where $\boldsymbol{\phi}_0 \in C_0^\infty(B; \mathbb{R}^m)$ and B is the unit ball in $\mathbb{R}^d$, we obtain

$$\lim_{\epsilon \to 0} \frac{\delta^2 I_\Omega(\boldsymbol{\phi}_\epsilon, \boldsymbol{0})}{\epsilon^d} = \int_B (L_{\boldsymbol{FF}}(\boldsymbol{x}_0)\nabla\boldsymbol{\phi}_0, \nabla\boldsymbol{\phi}_0))d\boldsymbol{x} \ge 0.$$

This condition is equivalent, via the density argument, to the inequality

$$\int_{\mathbb{R}^d} (L_{\boldsymbol{FF}}(\boldsymbol{x}_0)\nabla\boldsymbol{\phi}, \nabla\boldsymbol{\phi}))d\boldsymbol{x} \ge 0 \tag{7.2}$$

which must hold for all $\boldsymbol{\phi} \in H^1(\mathbb{R}^d; \mathbb{R}^m)$. Applying the Parceval's identity we obtain

$$\int_{\mathbb{R}^d} (L_{\boldsymbol{FF}}(\boldsymbol{x}_0)(\widehat{\boldsymbol{\phi}}(\boldsymbol{k}) \otimes \boldsymbol{k}), \widehat{\boldsymbol{\phi}}(\boldsymbol{k}) \otimes \boldsymbol{k})d\boldsymbol{k} \ge 0, \tag{7.3}$$

where $\widehat{\boldsymbol{\phi}}(\boldsymbol{k})$ is the Fourier transform of $\boldsymbol{\phi}(\boldsymbol{x})$. We conclude that (7.2) holds if and only if the acoustic tensor $\boldsymbol{A}(\boldsymbol{n})$ at $\boldsymbol{F}_0$ is non-negative definite for all directions $\boldsymbol{n}$. The acoustic tensor is a symmetric $m \times m$ matrix $\boldsymbol{A}(\boldsymbol{n})$ defined in terms of its quadratic form:

$$(\boldsymbol{A}(\boldsymbol{n})\boldsymbol{u}, \boldsymbol{u}) = (L_{\boldsymbol{FF}}(\boldsymbol{u} \otimes \boldsymbol{n}), \boldsymbol{u} \otimes \boldsymbol{n}). \tag{7.4}$$

In addition to the acoustic tensor $\boldsymbol{A}(\boldsymbol{n})$, let us define the 4-linear "acoustic form" described by an $m \times m$ matrix $\boldsymbol{A}(\boldsymbol{m}, \boldsymbol{n})$:

$$(\boldsymbol{A}(\boldsymbol{m}, \boldsymbol{n})\boldsymbol{u}, \boldsymbol{v}) = (L_{\boldsymbol{FF}}(\boldsymbol{u} \otimes \boldsymbol{m}), \boldsymbol{v} \otimes \boldsymbol{n}).$$

Then $\boldsymbol{A}(\boldsymbol{n}) = \boldsymbol{A}(\boldsymbol{n}, \boldsymbol{n})$ and $\boldsymbol{A}^T(\boldsymbol{m}, \boldsymbol{n}) = \boldsymbol{A}(\boldsymbol{n}, \boldsymbol{m})$. Let

$$\boldsymbol{\Gamma}(\boldsymbol{m}, \boldsymbol{n}) = (\boldsymbol{A}(\boldsymbol{m}, \boldsymbol{n}) + \boldsymbol{A}(\boldsymbol{n}, \boldsymbol{m}))/2, \quad \boldsymbol{\Lambda}(\boldsymbol{m}, \boldsymbol{n}) = (\boldsymbol{A}(\boldsymbol{m}, \boldsymbol{n}) - \boldsymbol{A}(\boldsymbol{n}, \boldsymbol{m}))/2$$

be the symmetric and antisymmetric parts of the acoustic form $\boldsymbol{A}(\boldsymbol{m}, \boldsymbol{n})$, respectively. Once the direction of the unit normal $\boldsymbol{n}$ is chosen, we denote with a subscript "+" the trace on the phase boundary from the region to which $\boldsymbol{n}$ points. The other trace is denoted with the subscript "−". The formulas that contain no + or − subscripts should be understood as two formulas for each of the two subscripts.

7.2 Localization of the second variation

Below we perform the general localization analysis, which is the direct analog of the classical Legendre-Hadamard analysis based on (7.1) and (7.3). Such analysis was first done by Grinfeld [28, 29] in the context of a special example.

We begin by choosing the same sequence of test functions $\boldsymbol{\phi}_\epsilon(\boldsymbol{x})$ and $\boldsymbol{\theta}_\epsilon(\boldsymbol{x})$ as in (7.1) and using them in the formula (3.19) to obtain the expression for $\delta^2 I_\Omega(\boldsymbol{\phi}, \boldsymbol{\theta})$. If $\boldsymbol{x}_0 \in \Sigma$ then by changing variables $\boldsymbol{x} = \boldsymbol{x}_0 + \epsilon \boldsymbol{z}$ we obtain

$$\lim_{\epsilon \to 0} \frac{\delta^2 I_\Omega(\boldsymbol{\phi}_\epsilon, \boldsymbol{\theta}_\epsilon)}{\epsilon^d} = \delta^2 I_{\text{loc}}(\boldsymbol{\phi}_0, \boldsymbol{\theta}_0). \tag{7.5}$$

The localized second variation $\delta^2 I_{\text{loc}}(\boldsymbol{\phi}_0, \boldsymbol{\theta}_0)$ retains the same form as the original general second variation $\delta^2 I_\Omega(\boldsymbol{\phi}, \boldsymbol{\theta})$, except the surface of discontinuity Σ is replaced by its tangent plane $T_{\boldsymbol{x}_0}\Sigma$ at $\boldsymbol{x}_0$ and $\boldsymbol{F}(\boldsymbol{x})$ is replaced with

$$\overline{\boldsymbol{F}}(\boldsymbol{z}) = \lim_{\epsilon \to 0} \boldsymbol{F}(\boldsymbol{x}_0 + \epsilon \boldsymbol{z}) = \begin{cases} \boldsymbol{F}_+, & \text{if } \boldsymbol{z} \cdot \boldsymbol{n} > 0 \\ \boldsymbol{F}_-, & \text{if } \boldsymbol{z} \cdot \boldsymbol{n} < 0. \end{cases} \tag{7.6}$$

Therefore, the same argument, leading from (3.19) to (5.16) holds and results in the formula

$$\delta^2 I_{\text{loc}}(\boldsymbol{\phi}_0, \boldsymbol{\theta}_0) = \int_B (L_{\boldsymbol{FF}}(\boldsymbol{z})\widetilde{\nabla}\boldsymbol{\psi}, \widetilde{\nabla}\boldsymbol{\psi})d\boldsymbol{z} - \int_{T_{\boldsymbol{x}_0}\Sigma \cap B} ([\![\boldsymbol{P}]\!], \nabla_\Sigma \{\!\!\{\boldsymbol{\psi}\}\!\!\})\xi(\boldsymbol{z})dS(\boldsymbol{z}),$$

where

$$L_{\boldsymbol{FF}}(\boldsymbol{z}) = L_{\boldsymbol{FF}}(\boldsymbol{x}_0, \boldsymbol{y}(\boldsymbol{x}_0), \overline{\boldsymbol{F}}(\boldsymbol{z})), \qquad \boldsymbol{\psi}(\boldsymbol{z}) = \boldsymbol{\phi}_0(\boldsymbol{z}) - \overline{\boldsymbol{F}}(\boldsymbol{z})\boldsymbol{\theta}_0(\boldsymbol{z}), \qquad \xi(\boldsymbol{z}) = (\boldsymbol{\theta}_0(\boldsymbol{z}), \boldsymbol{n}).$$

The remaining terms in (5.16) vanish in the limit (7.5), because the rescaled Lagrangian $L_{\text{loc}}(\boldsymbol{F}) = L(\boldsymbol{x}_0, \boldsymbol{y}(\boldsymbol{x}_0), \boldsymbol{F})$ does not depend on $\boldsymbol{x}$ and $\boldsymbol{y}$ explicitly and because the field $\overline{\boldsymbol{F}}(\boldsymbol{z})$ is piecewise constant.

The density argument, as in the classical case allows us to define the localized condition

$$\delta^2 I_{\text{loc}}(\boldsymbol{\psi}) = \int_{\mathbb{R}^d} (L_{\boldsymbol{FF}}(\boldsymbol{z})\widetilde{\nabla}\boldsymbol{\psi}, \widetilde{\nabla}\boldsymbol{\psi})d\boldsymbol{z} - \int_{\Pi_{\boldsymbol{n}}} ([\![\boldsymbol{P}]\!], \nabla_\Sigma \{\boldsymbol{\psi}\})\xi(\boldsymbol{z})dS(\boldsymbol{z}) \geq 0, \tag{7.7}$$

where $\Pi_{\boldsymbol{n}} = \{\boldsymbol{z} \in \mathbb{R}^d : (\boldsymbol{z}, \boldsymbol{n}) = 0\}$. The fields $\boldsymbol{\psi}_\pm \in C^1(\mathbb{H}_\pm; \mathbb{R}^m) \cap H^1(\mathbb{H}_\pm; \mathbb{R}^m)$ and $\xi \in C^1(\Pi_{\boldsymbol{n}}) \cap L^2(\Pi_{\boldsymbol{n}})$ satisfy

$$[\![\boldsymbol{\psi}]\!] = -\boldsymbol{a}\xi(\boldsymbol{z}), \tag{7.8}$$

where $\boldsymbol{a}$ is defined in (5.6) and

$$\mathbb{H}_\pm = \{\boldsymbol{z} \in \mathbb{R}^d : \pm(\boldsymbol{z}, \boldsymbol{n}) > 0\}.$$

Continuing the parallel with the classical Legendre-Hadamard condition we analyze the non-negativity of (7.7) by means of the Parceval's identity. The difference here is that Parceval's identity could be used only along the plane $\Pi_{\boldsymbol{n}}$ [1, 10]. In the normal direction, derivatives cannot be eliminated via a Fourier transform.

First we consider the bulk term

$$\int_{\mathbb{R}^d} (L_{\boldsymbol{FF}}(\boldsymbol{z})\widetilde{\nabla}\boldsymbol{\psi}, \widetilde{\nabla}\boldsymbol{\psi})d\boldsymbol{z} = B^+ + B^-,$$

where

$$B^\pm = \int_{\mathbb{H}_\pm} (L^\pm_{\boldsymbol{FF}}\nabla\boldsymbol{\psi}, \nabla\boldsymbol{\psi})d\boldsymbol{z}$$

Now we can apply the $d-1$-dimensional Parceval's identity along the plane $\Pi_{\boldsymbol{n}}$:

$$B^\pm = \int_0^\infty \int_{\Pi_{\boldsymbol{n}}} \Big\{(\boldsymbol{A}_\pm(\boldsymbol{m})\widehat{\boldsymbol{\psi}}_\pm, \widehat{\boldsymbol{\psi}}_\pm) + (\boldsymbol{A}_\pm(\boldsymbol{n})\widehat{\boldsymbol{\psi}'}_\pm, \widehat{\boldsymbol{\psi}'}_\pm) \pm 2\mathfrak{Im}(\boldsymbol{A}_\pm(\boldsymbol{m},\boldsymbol{n})\widehat{\boldsymbol{\psi}}_\pm, \widehat{\boldsymbol{\psi}'}_\pm)\Big\} đ\boldsymbol{m}dt,$$

where $(\cdot, \cdot)$ denotes the Hermitian inner product, and

$$đ\boldsymbol{m} = \frac{d\boldsymbol{m}}{(2\pi)^{d-1}} \tag{7.9}$$

is the normalized Lebesgue measure on $\Pi_{\boldsymbol{n}}$. Here we also introduced notations

$$\widehat{\boldsymbol{\psi}}(\boldsymbol{m}, t) = \int_{\Pi_{\boldsymbol{n}}} \boldsymbol{\psi}(\boldsymbol{z}', t)e^{i(\boldsymbol{m},\boldsymbol{z}')}d\boldsymbol{z}', \qquad \widehat{\boldsymbol{\psi}'}(\boldsymbol{m}, t) = \frac{\partial\widehat{\boldsymbol{\psi}}(\boldsymbol{m}, t)}{\partial t}, \qquad \boldsymbol{m} \in \Pi_{\boldsymbol{n}},$$

where $\boldsymbol{\psi}_\pm(\boldsymbol{z}',t)=\boldsymbol{\psi}(\boldsymbol{z}'\pm t\boldsymbol{n})$ for $\boldsymbol{z}'\in\Pi_{\boldsymbol{n}}$ and $t\in\mathbb{R}$.

Now, consider the surface term in (7.7). We obtain

$$\int_{\Pi_{\boldsymbol{n}}}\xi([\![\boldsymbol{P}]\!],\nabla_{\Pi_{\boldsymbol{n}}}\{\!\!\{\boldsymbol{\psi}\}\!\!\})d\boldsymbol{u}=i\int_{\Pi_{\boldsymbol{n}}}\widehat{\xi}([\![\boldsymbol{P}]\!]\boldsymbol{m},\{\!\!\{\widehat{\boldsymbol{\psi}}(0)\}\!\!\})đ\boldsymbol{m}=-\mathfrak{Im}\int_{\Pi_{\boldsymbol{n}}}\widehat{\xi}([\![\boldsymbol{P}]\!]\boldsymbol{m},\{\!\!\{\widehat{\boldsymbol{\psi}}(0)\}\!\!\})đ\boldsymbol{m},$$

where $\widehat{\boldsymbol{\psi}}(0)$ is the shorthand for $\widehat{\boldsymbol{\psi}}(\boldsymbol{m},0)$.

Next we split $\boldsymbol{A}(\boldsymbol{m},\boldsymbol{n})$ into symmetric and antisymmetric parts $\boldsymbol{A}(\boldsymbol{m},\boldsymbol{n})=\boldsymbol{\Gamma}(\boldsymbol{m},\boldsymbol{n})+\boldsymbol{\Lambda}(\boldsymbol{m},\boldsymbol{n})$ and observe that

$$\int_0^\infty 2\mathfrak{Im}(\boldsymbol{\Lambda}(\boldsymbol{m},\boldsymbol{n})\widehat{\boldsymbol{\psi}}(t),\widehat{\boldsymbol{\psi}'}(t))dt=-\mathfrak{Im}(\boldsymbol{\Lambda}(\boldsymbol{m},\boldsymbol{n})\widehat{\boldsymbol{\psi}}(0),\widehat{\boldsymbol{\psi}}(0)),$$

where $\widehat{\boldsymbol{\psi}}(t)$ is the shorthand for $\widehat{\boldsymbol{\psi}}(\boldsymbol{m},t)$. Thus,

$$\delta^2 I_{\rm loc}(\boldsymbol{\psi})=\int_{\Pi_{\boldsymbol{n}}}\left\{\mathcal{I}_0(\boldsymbol{m})+\int_0^\infty(\mathcal{I}^+(\widehat{\boldsymbol{\psi}}_+(t))+\mathcal{I}^-(\widehat{\boldsymbol{\psi}}_-(t)))dt\right\}đ\boldsymbol{m},$$

where

$$\mathcal{I}^\pm(\boldsymbol{f}(t))=(\boldsymbol{A}_\pm(\boldsymbol{m})\boldsymbol{f}(t),\boldsymbol{f}(t))+(\boldsymbol{A}_\pm(\boldsymbol{n})\boldsymbol{f}'(t),\boldsymbol{f}'(t))\pm 2\mathfrak{Im}(\boldsymbol{\Gamma}_\pm(\boldsymbol{m},\boldsymbol{n})\boldsymbol{f}(t),\boldsymbol{f}'(t))$$

and

$$\mathcal{I}_0(\boldsymbol{m})=-\mathfrak{Im}\left\{[\![(\boldsymbol{\Lambda}(\boldsymbol{m},\boldsymbol{n})\widehat{\boldsymbol{\psi}}(0),\widehat{\boldsymbol{\psi}}(0))]\!]-2\widehat{\xi}([\![\boldsymbol{P}]\!]\boldsymbol{m},\{\!\!\{\widehat{\boldsymbol{\psi}}(0)\}\!\!\})\right\}.$$

The problem now is for each fixed $\boldsymbol{m}\perp\boldsymbol{n}$ to minimize

$$\mathcal{J}(\boldsymbol{\psi})=\mathcal{I}_0(\boldsymbol{m})+\int_0^\infty\left(\mathcal{I}^+(\widehat{\boldsymbol{\psi}}_+(t))+\mathcal{I}^-(\widehat{\boldsymbol{\psi}}_-(t))\right)dt,$$

subject to the constraint

$$[\![\widehat{\boldsymbol{\psi}}(0)]\!]=-\widehat{\xi}\boldsymbol{a} \tag{7.10}$$

which is due to (7.8).

7.3 Auxiliary variational problem

The strategy is to solve first the auxiliary classical variational problem

$$\mathcal{I}^\pm_*(\boldsymbol{f}_0)=\min_{\boldsymbol{f}(0)=\boldsymbol{f}_0}\int_0^\infty\mathcal{I}^\pm(\boldsymbol{f}(t))dt. \tag{7.11}$$

The minimum $\mathcal{I}^\pm_*(\boldsymbol{f}_0)$ is going to be quadratic in $\boldsymbol{f}_0$. Then the non-negativity of $\delta^2 I_{\rm loc}(\boldsymbol{\psi})$ is going to be equivalent to the non-negativity of the quadratic form

$$q(\widehat{\boldsymbol{\psi}}_-(0),\widehat{\xi})=\mathcal{I}^+_*(\widehat{\boldsymbol{\psi}}_+(0))+\mathcal{I}^-_*(\widehat{\boldsymbol{\psi}}_-(0))+\mathcal{I}_0(\boldsymbol{m}), \tag{7.12}$$

where $\widehat{\boldsymbol{\psi}}_+(0)$ is eliminated from (7.12) via (7.10).

The Euler-Lagrange system for (7.11) is

$$\boldsymbol{A}_\pm(\boldsymbol{m})\boldsymbol{f}(t) - \boldsymbol{A}_\pm(\boldsymbol{n})\boldsymbol{f}''(t) \pm 2i\boldsymbol{\Gamma}_\pm(\boldsymbol{m},\boldsymbol{n})\boldsymbol{f}'(t) = 0. \tag{7.13}$$

We assume that the acoustic tensors $\boldsymbol{A}_\pm(\boldsymbol{n})$ are strictly positive definite for all $|\boldsymbol{n}| = 1$. Therefore, the second order system (7.13) can be rewritten as the first order system of twice the size:

$$\boldsymbol{f}'(t) = \boldsymbol{h}(t), \quad \boldsymbol{h}'(t) = \boldsymbol{M}\boldsymbol{f}(t) + i\boldsymbol{N}\boldsymbol{h}(t),$$

where the matrices $\boldsymbol{M}$ and $\boldsymbol{N}$ are given by

$$\boldsymbol{M}_\pm = \boldsymbol{A}_\pm(\boldsymbol{n})^{-1}\boldsymbol{A}_\pm(\boldsymbol{m}), \quad \boldsymbol{N}_\pm = \pm 2\boldsymbol{A}_\pm^{-1}(\boldsymbol{n})\boldsymbol{\Gamma}_\pm(\boldsymbol{m},\boldsymbol{n}). \tag{7.14}$$

In other words, if $\boldsymbol{u}(t) = (\boldsymbol{f}(t), \boldsymbol{h}(t))$ then $\boldsymbol{u}'(t) = \mathbb{K}\boldsymbol{u}(t)$, where $\mathbb{K}$ is given by

$$\mathbb{K} = \begin{bmatrix} \boldsymbol{0} & \boldsymbol{I} \\ \boldsymbol{M} & i\boldsymbol{N} \end{bmatrix}. \tag{7.15}$$

The solutions of this linear system of ODEs with constant coefficients come from the spectral data for $\mathbb{K}$. Suppose, $\lambda \in \mathbb{C}$ is an eigenvalue for $\mathbb{K}$ and $\boldsymbol{u}^\lambda = (\boldsymbol{f}^\lambda, \boldsymbol{h}^\lambda)$ is an eigenvector. Then

$$\boldsymbol{A}_\pm(\boldsymbol{m})\boldsymbol{f}^\lambda \pm 2i\lambda\boldsymbol{\Gamma}_\pm(\boldsymbol{m},\boldsymbol{n})\boldsymbol{f}^\lambda = \lambda^2\boldsymbol{A}_\pm(\boldsymbol{n})\boldsymbol{f}^\lambda.$$

Let us set $\lambda = i\tau$ and take a (Hermitian) inner product with $\boldsymbol{f}^\lambda$. We obtain

$$(\boldsymbol{A}_\pm(\boldsymbol{m})\boldsymbol{f}^\lambda, \boldsymbol{f}^\lambda) \pm 2\tau(\boldsymbol{\Gamma}_\pm(\boldsymbol{m},\boldsymbol{n})\boldsymbol{f}^\lambda, \boldsymbol{f}^\lambda) + \tau^2(\boldsymbol{A}_\pm(\boldsymbol{n})\boldsymbol{f}^\lambda, \boldsymbol{f}^\lambda) = 0.$$

This equation has no real roots, because the matrices

$$\boldsymbol{A}_\pm(\boldsymbol{m} \pm \tau\boldsymbol{n}) = \boldsymbol{A}_\pm(\boldsymbol{m}) \pm 2\tau\boldsymbol{\Gamma}_\pm(\boldsymbol{m},\boldsymbol{n}) + \tau^2\boldsymbol{A}_\pm(\boldsymbol{n})$$

are strictly positive definite by our assumption. Thus $\mathbb{K}$ has no purely imaginary eigenvalues. In addition, since the matrices $\boldsymbol{A}(\boldsymbol{m})$, $\boldsymbol{A}(\boldsymbol{n})$ and $\boldsymbol{\Gamma}(\boldsymbol{m},\boldsymbol{n})$ are real, if λ is an eigenvalue of $\mathbb{K}$, then so is $-\overline{\lambda}$. The fact that $\mathbb{K}$ has no purely imaginary eigenvalues implies that λ and $-\overline{\lambda}$ are distinct and thus $\mathbb{K}$ has the Jordan normal form given by

$$\mathbb{K} = \begin{bmatrix} \boldsymbol{C}_{11} & \boldsymbol{C}_{12} \\ \boldsymbol{C}_{21} & \boldsymbol{C}_{22} \end{bmatrix} \begin{bmatrix} \boldsymbol{J} & \boldsymbol{0} \\ \boldsymbol{0} & -\overline{\boldsymbol{J}} \end{bmatrix} \begin{bmatrix} \boldsymbol{C}_{11} & \boldsymbol{C}_{12} \\ \boldsymbol{C}_{21} & \boldsymbol{C}_{22} \end{bmatrix}^{-1}, \tag{7.16}$$

where the $m \times m$ block $\boldsymbol{J}$ corresponds to the eigenvalues with negative real parts.

For a given fixed $\boldsymbol{f}_0 \in \mathbb{C}^m$, we need to find $\boldsymbol{h}_0 \in \mathbb{C}^m$ such that $\boldsymbol{u}_0 = (\boldsymbol{f}_0, \boldsymbol{h}_0)$ belongs to the invariant subspace of $\mathbb{K}$ corresponding to the Jordan block $\boldsymbol{J}$, i.e. generating an exponentially decaying geodesic. It is not difficult to show that there is a unique choice of $\boldsymbol{h}_0$ given by $\boldsymbol{h}_0 = \boldsymbol{Q}\boldsymbol{f}_0$, where $\boldsymbol{Q} = \boldsymbol{C}_{21}\boldsymbol{C}_{11}^{-1}$ and the matrices $\boldsymbol{C}_{ij}$ are defined via the Jordan decomposition (7.16). Thus, for each $\boldsymbol{f}_0 \in \mathbb{C}^m$ there is a unique exponentially decaying geodesic $\boldsymbol{u}(t)$ such that $\boldsymbol{u}(0) = (\boldsymbol{f}_0, \boldsymbol{h}_0)$ for some $\boldsymbol{h}_0 \in \mathbb{C}^m$. It is easy to calculate that

$$\mathcal{I}_*^{\pm}(\boldsymbol{f}_0) = -(\boldsymbol{K}_{\pm}\boldsymbol{f}_0, \boldsymbol{f}_0),$$

where $\boldsymbol{K}$ is defined by

$$\boldsymbol{K}(\boldsymbol{m}, \boldsymbol{n}) = (\boldsymbol{A}(\boldsymbol{n})\boldsymbol{C}_{11}\boldsymbol{J}\boldsymbol{C}_{11}^{-1})^H = (\boldsymbol{A}(\boldsymbol{n})\boldsymbol{Q})^H, \tag{7.17}$$

where $\boldsymbol{X}^H = (\boldsymbol{X} + \boldsymbol{X}^*)/2$ is the Hermitian symmetrization of $\boldsymbol{X}$ ($\boldsymbol{X}^*$ denotes the usual Hermitian adjoint).

There is a way to compute $\boldsymbol{Q}$ in (7.17) without having to compute the Jordan decomposition (7.16) of $\mathbb{K}$. Let $p_{\boldsymbol{J}}(\lambda)$ be the characteristic polynomial of $\boldsymbol{J}$. Multiplying (7.16) by

$$\begin{bmatrix} \boldsymbol{C}_{11} & \boldsymbol{C}_{12} \\ \boldsymbol{C}_{21} & \boldsymbol{C}_{22} \end{bmatrix}$$

on the right and expanding, we obtain, after easy manipulations, that (see also [42])

$$\boldsymbol{M} + i\boldsymbol{N}\boldsymbol{Q} = \boldsymbol{Q}^2. \tag{7.18}$$

By the Cayley-Hamilton theorem $p_{\boldsymbol{J}}(\boldsymbol{Q}) = \boldsymbol{0}$. The equation (7.18) can then be used to reduce this polynomial equation to the linear equation of the form $\boldsymbol{U}\boldsymbol{Q} = \boldsymbol{V}$, which is easily solvable for $\boldsymbol{Q}$. For example, If $m = 2$ and $p_{\boldsymbol{J}}(\lambda) = \lambda^2 - a_1\lambda + a_2$ then

$$(a_1\boldsymbol{I} - i\boldsymbol{N})\boldsymbol{Q} = \boldsymbol{M} + a_2\boldsymbol{I}. \tag{7.19}$$

If $m = 3$ and $p_{\boldsymbol{J}}(\lambda) = \lambda^3 - a_1\lambda^2 + a_2\lambda - a_3$, then, we get

$$(\boldsymbol{M} - \boldsymbol{N}^2 - ia_1\boldsymbol{N} + a_2\boldsymbol{I})\boldsymbol{Q} = a_1\boldsymbol{M} + a_3\boldsymbol{I} - i\boldsymbol{N}\boldsymbol{M}. \tag{7.20}$$

Observe that the characteristic polynomial $P_{\mathbb{K}}(\lambda)$ of $\mathbb{K}$ has the structure

$$P_{\mathbb{K}}(\lambda) = (-1)^m p_{\boldsymbol{J}}(\lambda)\overline{p_{\boldsymbol{J}}(-\overline{\lambda})}.$$

If $\lambda = i\tau$, $\tau \in \mathbb{R}$ then

$$P_{\mathbb{K}_{\pm}}(i\tau) = (-1)^m \frac{\det \boldsymbol{A}_{\pm}(\boldsymbol{m} \mp \tau\boldsymbol{n})}{\det \boldsymbol{A}_{\pm}(\boldsymbol{n})}.$$

Thus, the characteristic polynomial $p_{\boldsymbol{J}}(\lambda)$ of $\boldsymbol{J}$ can be computed from the equation

$$|p_{\boldsymbol{J}_{\pm}}(i\tau)|^2 = \frac{\det \boldsymbol{A}_{\pm}(\boldsymbol{m} \mp \tau\boldsymbol{n})}{\det \boldsymbol{A}_{\pm}(\boldsymbol{n})}, \quad \tau \in \mathbb{R}.$$

To do this, one needs to compute the roots of

$$\det \boldsymbol{A}_{\pm}(\boldsymbol{m} \mp \tau\boldsymbol{n}) = 0, \tag{7.21}$$

which come as a set of m complex-conjugate pairs. Then

$$p_{\boldsymbol{J}}(\lambda) = \prod_{j=1}^{m}(\lambda - i\tau_j),$$

where $\tau_1, \ldots, \tau_m$ are the roots of (7.21) with positive imaginary parts.

7.4 Algebraic form

We can now return to (7.12) and obtain

$$q(\{\widehat{\boldsymbol{\psi}}(0)\},\widehat{\xi}) = -\left(\begin{bmatrix} \mathsf{A}(\boldsymbol{m},\boldsymbol{n}) & \boldsymbol{p}(\boldsymbol{m},\boldsymbol{n}) \\ \overline{\boldsymbol{p}(\boldsymbol{m},\boldsymbol{n})} & \alpha(\boldsymbol{m},\boldsymbol{n}) \end{bmatrix} \begin{bmatrix} 2\{\widehat{\boldsymbol{\psi}}(0)\} \\ \widehat{\xi} \end{bmatrix}, \begin{bmatrix} 2\{\widehat{\boldsymbol{\psi}}(0)\} \\ \widehat{\xi} \end{bmatrix}\right),$$

where $\mathsf{A}(\boldsymbol{m},\boldsymbol{n})$, $\boldsymbol{p}(\boldsymbol{m},\boldsymbol{n})$ and $\alpha(\boldsymbol{m},\boldsymbol{n})$ are given by

$$\mathsf{A}(\boldsymbol{m},\boldsymbol{n}) = -\frac{i}{2}[\![\boldsymbol{\Lambda}(\boldsymbol{m},\boldsymbol{n})]\!] + \{\boldsymbol{K}(\boldsymbol{m},\boldsymbol{n})\}, \tag{7.22}$$

$$\boldsymbol{p}(\boldsymbol{m},\boldsymbol{n}) = -i[\![\boldsymbol{P}]\!]\boldsymbol{m} + \left(-i\{\boldsymbol{\Lambda}(\boldsymbol{m},\boldsymbol{n})\} + \frac{1}{2}[\![\boldsymbol{K}(\boldsymbol{m},\boldsymbol{n})]\!]\right)[\![\boldsymbol{F}]\!]\boldsymbol{n} \tag{7.23}$$

and

$$\alpha(\boldsymbol{m},\boldsymbol{n}) = (\{\boldsymbol{K}(\boldsymbol{m},\boldsymbol{n})\}[\![\boldsymbol{F}]\!]\boldsymbol{n}, [\![\boldsymbol{F}]\!]\boldsymbol{n}). \tag{7.24}$$

Using our analysis it is now straightforward to construct the perturbation $(\boldsymbol{\psi}(\boldsymbol{x}), \xi(\boldsymbol{z}'))$ corresponding to any given vector $([\![\widehat{\boldsymbol{\psi}}(0)]\!], \widehat{\xi})$. Hence, the condition

$$\mathbb{A}(\boldsymbol{m},\boldsymbol{n}) = -\begin{bmatrix} \mathsf{A}(\boldsymbol{m},\boldsymbol{n}) & \boldsymbol{p}(\boldsymbol{m},\boldsymbol{n}) \\ \overline{\boldsymbol{p}(\boldsymbol{m},\boldsymbol{n})} & \alpha(\boldsymbol{m},\boldsymbol{n}) \end{bmatrix} \geq 0 \tag{7.25}$$

implies the non-negativity of $\delta^2 I_{\text{loc}}$.

Our analysis involves localized variations of Euler-Lagrange type leading to the Legendre-Hadamard condition in the absence of discontinuities. For this reason we call the matrix $\mathbb{A}$ the *phase boundary acoustic tensor*. Since the phase boundary acoustic tensor $\mathbb{A}(\boldsymbol{m},\boldsymbol{n})$ is given in block form, it makes sense to reformulate the condition of non-negative definiteness of $\mathbb{A}(\boldsymbol{m},\boldsymbol{n})$ in terms of its blocks. A simple linear algebra gives the following result.

THEOREM **7.1.** *Suppose that the uniform Legendre-Hadamard condition $\boldsymbol{A}_{\pm}(\boldsymbol{n}) > 0$ is satisfied for all $\boldsymbol{n}$. Then the second variation (7.7) is non-negative if and only if the matrix $\mathbb{A}(\boldsymbol{m},\boldsymbol{n})$ is positive semi-definite. The matrix $\mathbb{A}(\boldsymbol{m},\boldsymbol{n})$ is positive semi-definite if and only if $-\mathsf{A}(\boldsymbol{m},\boldsymbol{n})$ is a positive semi-definite matrix, $\boldsymbol{p}(\boldsymbol{m},\boldsymbol{n})$ belongs to the range of $\mathsf{A}(\boldsymbol{m},\boldsymbol{n})$ and*

$$\min_{\boldsymbol{m}\in\Pi_{\boldsymbol{n}},|\boldsymbol{m}|=1} \left\{(\mathsf{A}^{-1}(\boldsymbol{m},\boldsymbol{n})\boldsymbol{p}(\boldsymbol{m},\boldsymbol{n}), \boldsymbol{p}(\boldsymbol{m},\boldsymbol{n})) - \alpha(\boldsymbol{m},\boldsymbol{n})\right\} \geq 0, \tag{7.26}$$

where the inverse A^{-1} is taken on the range of A.

We remark that the condition

$$\mathsf{A}(\boldsymbol{m},\boldsymbol{n}) \leq 0, \qquad \boldsymbol{m} \perp \boldsymbol{n} \tag{7.27}$$

is equivalent to the Simpson-Spector condition [53], corresponding to the case $\boldsymbol{\theta} = \boldsymbol{0}$. In other words (7.27) is equivalent to the non-negativity of the classical outer second variation

$\delta^2 I_\Omega(\boldsymbol{\phi}, \mathbf{0})$. In that respect the condition (7.27) is a necessary condition for the classical weak local minimum, while condition (6.6) is necessary for the classical strong local minimum. Observe that the condition (7.27) is a constraint on the elastic moduli and the interface normal $\boldsymbol{n}$. It does not place any constraints on the values of deformation gradient $\boldsymbol{F}_\pm$ in contrast to the inequality (7.26).

Remark 7.2. *In the special case when $d = 2$ there is no minimum to compute in (7.26) and we can write explicitly*

$$(\mathsf{A}^{-1}(\boldsymbol{n}^\perp, \boldsymbol{n})\boldsymbol{p}(\boldsymbol{n}^\perp, \boldsymbol{n}), \boldsymbol{p}(\boldsymbol{n}^\perp, \boldsymbol{n})) \geq \alpha(\boldsymbol{n}^\perp, \boldsymbol{n}), \tag{7.28}$$

where $\boldsymbol{n}^\perp = (-n_2, n_1)$.

Remark 7.3. *What we have done for jump discontinuities could also apply to the traction part of the outer boundary of $\partial\Omega$. The respective calculations are a lot simpler, since inner variations are no longer allowed (unless we change the notion of a local minimum and allow variable reference domain.) The corresponding condition says that the $m \times m$ complex Hermitian matrices*

$$\mathsf{A}^b(\boldsymbol{m}, \boldsymbol{n}) = -i\boldsymbol{\Lambda}(\boldsymbol{m}, \boldsymbol{n}) - \boldsymbol{K}(\boldsymbol{m}, \boldsymbol{n}) \tag{7.29}$$

must be positive semi-definite for all $\boldsymbol{m} \perp \boldsymbol{n}$, where $\boldsymbol{n}$ is now the outer *unit normal to $\partial\Omega$.*

We will call the matrix $\mathsf{A}^b(\boldsymbol{\xi}, \boldsymbol{n})$ the *boundary acoustic tensor*. The Legendre-Hadamard condition for traction free boundaries have been discussed in detail in [42, 51, 52], where the authors also address the special case of quadratic energy and derived conditions that ensure non-negativity in the case when the acoustic tensor is not strictly positive definite.

7.5 Example

In this example we present a configuration satisfying (4.14) and (4.15), with positive definite classical second variation, whose instability is detected by the local condition (7.28).

Consider the scalar 2D variational problem, corresponding to anti-plane shear in elasticity with $d = 2$ and $m = 1$. The elastic energy has the form $L(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{F}) = W(\boldsymbol{F})$, where

$$W(\boldsymbol{F}) = \min\left\{\frac{1}{2}\mu_+|\boldsymbol{F}|^2 + w_+, \frac{1}{2}\mu_-|\boldsymbol{F}|^2 + w_-\right\}, \tag{7.30}$$

where $\boldsymbol{F} \in \mathbb{R}^2$ and $\mu_\pm > 0$ are the shear moduli of the phases. More specifically, if the transformation strains $\boldsymbol{F}^\circ_\pm$ are present, they can be again eliminated by a simple affine transformation. If

$$\widehat{W}(\boldsymbol{F}) = \min\left\{\frac{1}{2}\mu_+|\boldsymbol{F} - \boldsymbol{F}^\circ_+|^2 + \widehat{w}_+, \frac{1}{2}\mu_-|\boldsymbol{F} - \boldsymbol{F}^\circ_-|^2 + \widehat{w}_-\right\},$$

then

$$\widehat{W}(\boldsymbol{F}) = W(\boldsymbol{F} - \overline{\boldsymbol{F}}) + (\boldsymbol{\sigma}^\circ, \boldsymbol{F}) - \frac{1}{2}(\boldsymbol{\sigma}^\circ, \overline{\boldsymbol{F}}),$$

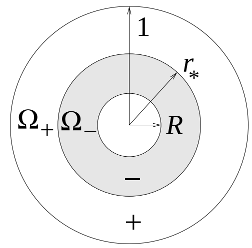

Figure 4: The heterogeneous annulus.

where
$$\overline{\boldsymbol{F}} = \frac{[\![\mu \boldsymbol{F}^\circ]\!]}{[\![\mu]\!]}, \qquad \boldsymbol{\sigma}^\circ = \{\!\{\mu\}\!\}\overline{\boldsymbol{F}} - \{\!\{\mu \boldsymbol{F}^\circ\}\!\}, \qquad w_\pm = \widehat{w}_\pm - \frac{1}{2}(\boldsymbol{\sigma}^\circ, \boldsymbol{F}^\circ_\pm).$$

We begin by computing the 2×2 matrix $\mathbb{A}(\boldsymbol{n}^\perp, \boldsymbol{n})$ for the energy (7.30). We have
$$M = 1, \qquad N = 0, \qquad Q = -\sqrt{M} = -1.$$
Therefore, $K(\boldsymbol{n}^\perp, \boldsymbol{n}) = -\mu$ and $\Lambda(\boldsymbol{n}^\perp, \boldsymbol{n}) = 0$. Hence, $\mathsf{A}(\boldsymbol{n}^\perp, \boldsymbol{n}) = -\{\!\{\mu\}\!\} < 0$. This shows that the condition (7.27) is satisfied regardless the orientation of the surface of discontinuity. We also have
$$p(\boldsymbol{n}^\perp, \boldsymbol{n}) = -i([\![\boldsymbol{P}]\!], \boldsymbol{n}^\perp) + \frac{1}{2}[\![\mu]\!]([\![\boldsymbol{F}]\!], \boldsymbol{n}).$$
and
$$\alpha(\boldsymbol{n}^\perp, \boldsymbol{n}) = -\{\!\{\mu\}\!\}([\![\boldsymbol{F}]\!], \boldsymbol{n})^2.$$
The inequality (7.28) is then equivalent to
$$\mu_+\mu_-([\![\boldsymbol{F}]\!], \boldsymbol{n})^2 \ge ([\![\boldsymbol{P}]\!], \boldsymbol{n}^\perp)^2. \tag{7.31}$$

Consider a circular annulus shown in Figure 4 and assume that the loading is compatible with the following equilibrium configuration
$$u(\boldsymbol{x}) = \begin{cases} (\boldsymbol{a}_-, \boldsymbol{x}) + \dfrac{(\boldsymbol{b}_-, \boldsymbol{x})}{r^2}, & \text{if } R \le |\boldsymbol{x}| \le r_* \\[2ex] (\boldsymbol{a}_+, \boldsymbol{x}) + \dfrac{(\boldsymbol{b}_+, \boldsymbol{x})}{r^2}, & \text{if } r_* \le |\boldsymbol{x}| \le 1 \end{cases} \tag{7.32}$$
The continuity of displacements and tractions can be written as
$$[\![\boldsymbol{a}]\!] + \frac{[\![\boldsymbol{b}]\!]}{r_*^2} = \boldsymbol{0}, \qquad [\![\mu \boldsymbol{a}]\!] = \frac{[\![\mu \boldsymbol{b}]\!]}{r_*^2}, \tag{7.33}$$
respectively. The Maxwell condition can be written as
$$p^* = \frac{1}{2}([\![\mu \boldsymbol{F}]\!], \{\!\{\boldsymbol{F}\}\!\}) - \frac{1}{2}([\![\boldsymbol{F}]\!], \{\!\{\mu \boldsymbol{F}\}\!\}) + [\![w]\!].$$

Knowing that the deformation gradient is equal to

$$\boldsymbol{F} = \boldsymbol{a} + (\boldsymbol{I} - 2\widehat{\boldsymbol{x}} \otimes \widehat{\boldsymbol{x}})\frac{\boldsymbol{b}}{r^2}.$$

We get from (7.33)

$$[\![\boldsymbol{F}]\!] = 2([\![\boldsymbol{a}]\!], \widehat{\boldsymbol{x}})\hat{\boldsymbol{x}}, \qquad [\![\mu \boldsymbol{F}]\!] = 2(\boldsymbol{I} - \widehat{\boldsymbol{x}} \otimes \widehat{\boldsymbol{x}})[\![\mu \boldsymbol{a}]\!].$$

Applying the product rule (5.5)

$$[\![\mu \boldsymbol{b}]\!] = [\![\mu]\!]\{\!\!\{\boldsymbol{b}\}\!\!\} + \{\!\!\{\mu\}\!\!\}[\![\boldsymbol{b}]\!], \qquad [\![\boldsymbol{b}]\!] = [\![\mu^{-1}\mu \boldsymbol{b}]\!] = [\![\mu^{-1}]\!]\{\!\!\{\mu \boldsymbol{b}\}\!\!\} + \{\!\!\{\mu^{-1}\}\!\!\}[\![\mu \boldsymbol{b}]\!]$$

and using (7.33) we can write

$$\frac{\{\!\!\{\boldsymbol{b}\}\!\!\}}{r_*^2} = \frac{[\![\mu \boldsymbol{a}]\!] + \{\!\!\{\mu\}\!\!\}[\![\boldsymbol{a}]\!]}{[\![\mu]\!]}, \qquad \frac{\{\!\!\{\mu \boldsymbol{b}\}\!\!\}}{r_*^2} = -\frac{[\![\boldsymbol{a}]\!] + \{\!\!\{\mu^{-1}\}\!\!\}[\![\mu \boldsymbol{a}]\!]}{[\![\mu^{-1}]\!]}.$$

Then, applying the product rule (5.5) again, we get

$$\{\!\!\{\boldsymbol{F}\}\!\!\} = \frac{2[\![\mu \boldsymbol{a}]\!]}{[\![\mu]\!]} - \frac{2}{[\![\mu]\!]}([\![\mu \boldsymbol{a}]\!] + \{\!\!\{\mu\}\!\!\}[\![\boldsymbol{a}]\!], \widehat{\boldsymbol{x}})\widehat{\boldsymbol{x}},$$

$$\{\!\!\{\mu \boldsymbol{F}\}\!\!\} = \frac{2[\![\boldsymbol{a}]\!]}{[\![\mu^{-1}]\!]} - \frac{2}{[\![\mu^{-1}]\!]}(\boldsymbol{I} - \widehat{\boldsymbol{x}} \otimes \widehat{\boldsymbol{x}})([\![\boldsymbol{a}]\!] + \{\!\!\{\mu^{-1}\}\!\!\}[\![\mu \boldsymbol{a}]\!]).$$

Hence,

$$p^* = \frac{2}{[\![\mu]\!]}((\boldsymbol{I} - \widehat{\boldsymbol{x}} \otimes \widehat{\boldsymbol{x}})[\![\mu \boldsymbol{a}]\!], [\![\mu \boldsymbol{a}]\!]) - \frac{2}{[\![\mu^{-1}]\!]}([\![\boldsymbol{a}]\!], \widehat{\boldsymbol{x}})^2 + [\![w]\!].$$

Let

$$\boldsymbol{B} = \frac{[\![\mu \boldsymbol{a}]\!] \otimes [\![\mu \boldsymbol{a}]\!]}{[\![\mu]\!]} + \frac{[\![\boldsymbol{a}]\!] \otimes [\![\boldsymbol{a}]\!]}{[\![\mu^{-1}]\!]}.$$

Then $p^* = 0$ is equivalent to $(\boldsymbol{B}\widehat{\boldsymbol{x}}, \widehat{\boldsymbol{x}}) = \beta$ for all $\widehat{\boldsymbol{x}}$, where

$$\beta = \frac{|[\![\mu \boldsymbol{a}]\!]|^2}{[\![\mu]\!]} + \frac{1}{2}[\![w]\!].$$

We conclude that $\boldsymbol{B} = \beta \boldsymbol{I}$. Observe also that for any vector $\boldsymbol{v} \in \mathbb{R}^2$ that is perpendicular to $[\![\boldsymbol{a}]\!]$ we get $(\boldsymbol{B}\boldsymbol{v}, \boldsymbol{v}) \geq 0$, assuming $\mu_+ > \mu_-$. Similarly for any vector $\boldsymbol{w} \in \mathbb{R}^2$ that is perpendicular to $[\![\mu \boldsymbol{a}]\!]$ we get $(\boldsymbol{B}\boldsymbol{w}, \boldsymbol{w}) \leq 0$. Hence $\det \boldsymbol{B} \leq 0$. But $\boldsymbol{B}$ is a multiple of the identity. Hence, we conclude that $\boldsymbol{B} = \boldsymbol{0}$ and $\beta = 0$. That means, that

$$[\![\mu \boldsymbol{a}]\!] = \nu [\![\boldsymbol{a}]\!], \quad \nu^2 = \mu_+\mu_-, \qquad |[\![\boldsymbol{a}]\!]|^2 = \frac{1}{2}[\![\mu^{-1}]\!][\![w]\!]. \tag{7.34}$$

We have in view of (7.33)

$$([\![\boldsymbol{F}]\!], \boldsymbol{n}) = 2([\![\boldsymbol{a}]\!], \widehat{\boldsymbol{x}}), \qquad ([\![\boldsymbol{P}]\!], \boldsymbol{n}^\perp) = 2([\![\mu \boldsymbol{a}]\!], \widehat{\boldsymbol{x}}^\perp) = 2\nu([\![\boldsymbol{a}]\!], \widehat{\boldsymbol{x}}^\perp).$$

If (7.31) holds then for any unit vector $\widehat{\boldsymbol{x}}$ we must have

$$4\mu_+\mu_-([\![\boldsymbol{a}]\!], \widehat{\boldsymbol{x}})^2 \geq 4\mu_+\mu_-([\![\boldsymbol{a}]\!], \widehat{\boldsymbol{x}}^\perp)^2.$$

According to (7.34), $[\![\boldsymbol{a}]\!] \neq \boldsymbol{0}$. Then taking $\widehat{\boldsymbol{x}} = [\![\boldsymbol{a}]\!]^\perp/|[\![\boldsymbol{a}]\!]|$, we obtain $|[\![\boldsymbol{a}]\!]|^2 = 0$ contradicting (7.34). We can now conclude that any solution $\boldsymbol{u}(\boldsymbol{x})$ in the annulus of the form (7.32) is unstable.

We remark that once the direction of $[\![\boldsymbol{a}]\!]$ is chosen arbitrarily, the solution (7.32) is determined uniquely by the jump conditions (7.33) and (7.34). Any such solution has positive classical second variation:

$$\delta^2 I_\Omega(\phi, \boldsymbol{0}) = \int_\Omega \mu(\boldsymbol{x})|\nabla\phi|^2 d\boldsymbol{x} > 0, \qquad \mu(\boldsymbol{x}) = \begin{cases} \mu_+, & R \leq |\boldsymbol{x}| \leq r_* \\ \mu_-, & r_* \leq |\boldsymbol{x}| \leq 1. \end{cases}$$

Remark 7.4. *The instability of solutions (7.32) could also be easily detected by the roughening stability condition derived in [26]. For this example it reads*

$$4\nu([\![\boldsymbol{a}]\!], \widehat{\boldsymbol{x}}^\perp)([\![\boldsymbol{a}]\!], \widehat{\boldsymbol{x}})\widehat{\boldsymbol{x}}^\perp = \boldsymbol{0}$$

for any unit vector $\widehat{\boldsymbol{x}}$. In other words, at least one component of $[\![\boldsymbol{a}]\!]$ must be zero in any orthonormal basis. This means that $[\![\boldsymbol{a}]\!] = \boldsymbol{0}$, contradicting (7.34).

Acknowledgments. This material is based upon work supported by the National Science Foundation under Grant No. 0707582. LT was also supported by the EU contract MRTN-CT-2004-505226. VK was partially supported by the Russian Foundation for Basic Research grant 10-01-00670-a.

A Grinfeld's expression for second variation

In [28, 29] Grinfeld considered the problem of stability of phase boundaries and computed the second variation of the energy for the case when the outer variation in the bulk regions is complemented by the simultaneous displacement of the phase boundary in Lagrangian coordinates. Although he did not use the concept of inner variations we can show that his result agrees with our formula (5.16), when $L(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{F}) = W(\boldsymbol{F})$.

Written in our notations, Grinfeld's second variation formula has the form $\delta^2 I_\Omega(\boldsymbol{\phi}, \boldsymbol{\theta}) = \delta^2 I_\Omega(\boldsymbol{\psi}, \boldsymbol{0}) - Z$, where $\boldsymbol{\psi}$ is given by (2.11) and

$$Z = \int_\Sigma \{\xi(\delta_{jk} - n_j n_k)[\![P_{ij}\psi_{i,k} - P_{ij,k}\psi_i]\!] + \xi^2(\delta_{jk} - n_j n_k)[\![P_{ij}F_{ik,r}]\!]n_r - [\![P_{ij}\psi_i]\!](\nabla_\Sigma\xi)_j\}dS.$$

Here we show that $Z = \mathfrak{S}$. Expanding and using the chain rule $P_{ij}F_{ij,r} = W_{,r}$, we get

$$Z = \int_\Sigma \{\xi[\![(\boldsymbol{P}, \nabla\boldsymbol{\psi})]\!] - \xi\left([\![\frac{\partial\boldsymbol{\psi}}{\partial\boldsymbol{n}}]\!], \boldsymbol{P}\boldsymbol{n}\right) + \xi[\![\left(\frac{\partial\boldsymbol{P}}{\partial\boldsymbol{n}}\boldsymbol{n}, \boldsymbol{\psi}\right)]\!] + \xi^2[\![\frac{\partial W}{\partial\boldsymbol{n}}]\!] - \xi^2\left(\boldsymbol{P}\boldsymbol{n}, [\![\frac{\partial\boldsymbol{F}}{\partial\boldsymbol{n}}]\!]\boldsymbol{n}\right) - \left([\![\boldsymbol{P}^T\boldsymbol{\psi}]\!], \nabla_\Sigma\xi\right)\}dS(\boldsymbol{x}).$$

Observe that

$$[\![(\boldsymbol{P},\nabla\boldsymbol{\psi})]\!]-\left([\![\frac{\partial\boldsymbol{\psi}}{\partial\boldsymbol{n}}]\!],\boldsymbol{P}\boldsymbol{n}\right)=[\![(\boldsymbol{P},\nabla_\Sigma\boldsymbol{\psi})]\!].$$

Using (5.22) for the third term in Z and integration by parts formula (5.21) in the last term in Z, we obtain

$$Z=\int_\Sigma\left\{2\xi[\![(\boldsymbol{P},\nabla_\Sigma\boldsymbol{\psi})]\!]+\xi^2[\![\frac{\partial W}{\partial\boldsymbol{n}}]\!]-\xi^2\left(\boldsymbol{P}\boldsymbol{n},[\![\frac{\partial\boldsymbol{F}}{\partial\boldsymbol{n}}]\!]\boldsymbol{n}\right)-\xi\left(\boldsymbol{P}\boldsymbol{n},[\![\boldsymbol{\psi}]\!]\right)\nabla_\Sigma\cdot\boldsymbol{n}\right\}dS(\boldsymbol{x}).$$

Now, let us apply the formula

$$[\![(\boldsymbol{P},\nabla_\Sigma\boldsymbol{\psi})]\!]=([\![\boldsymbol{P}]\!],\nabla_\Sigma\{\!\!\{\boldsymbol{\psi}\}\!\!\})+(\{\!\!\{\boldsymbol{P}\}\!\!\},\nabla_\Sigma[\![\boldsymbol{\psi}]\!])\tag{A.1}$$

and (5.9) to the first and the last terms of Z, respectively, to get

$$Z=\int_\Sigma\{2\xi([\![\boldsymbol{P}]\!],\nabla_\Sigma\{\!\!\{\boldsymbol{\psi}\}\!\!\})-2\xi(\{\!\!\{\boldsymbol{P}\}\!\!\},\nabla_\Sigma(\xi[\![\boldsymbol{F}]\!]\boldsymbol{n}))+\xi^2[\![\frac{\partial W}{\partial\boldsymbol{n}}]\!]$$
$$-\xi^2\left(\boldsymbol{P}\boldsymbol{n},[\![\frac{\partial\boldsymbol{F}}{\partial\boldsymbol{n}}]\!]\boldsymbol{n}\right)+\xi^2\left(\boldsymbol{P}\boldsymbol{n},[\![\boldsymbol{F}]\!]\boldsymbol{n}\right)\nabla_\Sigma\cdot\boldsymbol{n}\}dS(\boldsymbol{x}).$$

Let us apply (5.19) to the second term

$$Z'=-2\int_\Sigma\xi(\{\!\!\{\boldsymbol{P}\}\!\!\},\nabla_\Sigma(\xi[\![\boldsymbol{F}]\!]\boldsymbol{n}))dS(\boldsymbol{x})$$

of Z. We get

$$Z'=\int_\Sigma\left\{-(\{\!\!\{\boldsymbol{P}\}\!\!\}\nabla_\Sigma(\xi^2),[\![\boldsymbol{F}]\!]\boldsymbol{n})-2\xi^2\left(\{\!\!\{\boldsymbol{P}\}\!\!\},[\![\frac{\partial\boldsymbol{F}}{\partial\boldsymbol{n}}]\!]\right)+2\xi^2\left(\boldsymbol{P}\boldsymbol{n},[\![\frac{\partial\boldsymbol{F}}{\partial\boldsymbol{n}}]\!]\boldsymbol{n}\right)\right\}dS(\boldsymbol{x}).$$

Integrating the first term by parts and using (5.19) and (5.22) again, we obtain

$$Z'=\int_\Sigma\left\{\xi^2\left(\{\!\!\{\boldsymbol{P}\}\!\!\},[\![\frac{\partial\boldsymbol{F}}{\partial\boldsymbol{n}}]\!](\boldsymbol{I}-\boldsymbol{n}\otimes\boldsymbol{n})\right)-\xi^2\left(\{\!\!\{\frac{\partial\boldsymbol{P}}{\partial\boldsymbol{n}}\}\!\!\}\boldsymbol{n},[\![\boldsymbol{F}]\!]\boldsymbol{n}\right)-\xi^2(\boldsymbol{P}\boldsymbol{n},[\![\boldsymbol{F}]\!]\boldsymbol{n})\nabla_\Sigma\cdot\boldsymbol{n}\right.$$
$$\left.-2\xi^2\left(\{\!\!\{\boldsymbol{P}\}\!\!\},[\![\frac{\partial\boldsymbol{F}}{\partial\boldsymbol{n}}]\!]\right)+2\xi^2\left(\boldsymbol{P}\boldsymbol{n},[\![\frac{\partial\boldsymbol{F}}{\partial\boldsymbol{n}}]\!]\boldsymbol{n}\right)\right\}dS(\boldsymbol{x}).$$

Now we substitute this expression for Z' back into the formula for Z and use (5.6). After all the cancellations we obtain

$$Z=\int_\Sigma\left\{2\xi([\![\boldsymbol{P}]\!],\nabla_\Sigma\{\!\!\{\boldsymbol{\psi}\}\!\!\})+\xi^2[\![\frac{\partial W}{\partial\boldsymbol{n}}]\!]-\xi^2\left(\{\!\!\{\frac{\partial\boldsymbol{P}}{\partial\boldsymbol{n}}\}\!\!\},[\![\boldsymbol{F}]\!]\right)-\xi^2\left(\{\!\!\{\boldsymbol{P}\}\!\!\},[\![\frac{\partial\boldsymbol{F}}{\partial\boldsymbol{n}}]\!]\right)\right\}dS(\boldsymbol{x}),$$

which agrees with the surface integral term in (5.16) in view of (5.17).

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